QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 01

1. Which of the following is the correct order for He^+.

   (a) 3s < 3p < 3d (b) 3p < 3s < 3d (c) 3s > 3p > 3d (d) 3s = 3p = 3d

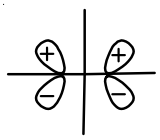
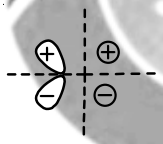
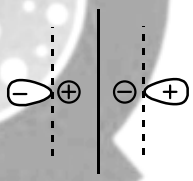
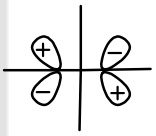
2. Number of degenerate orbitals in the 4th energy level of He and He^+ are

   (a) 16 and 1 (b) 1 and 16 (c) 9 and 1 (d) 1 and 9

3. d_{z^2} orbital has:

   (a) Four lobes (b) Two nodal planes (c) No nodes (d) Two conical nodes

4. Select the correct diagram for the π^* $2p_y$-orbital:

   (a)  (b)  (c)  (d) 

5. Which pair of orbitals show differential shielding?

   (a) d_{xy}, d_{yz} (b) $d_{z^2}, d_{x^2-y^2}$ (c) $d_{xz}, d_{x^2-y^2}$ (d) All of these

6. Which the following interaction form nonbonding molecular orbital when z-axis is the bonding axis ?

   (a) $d_{yz} + d_{z^2}$ (b) $d_{yz} + d_{xy}$

   (c) $d_{x^2-y^2} + d_{xy}$ (d) All form N.B.M.O.

7. Which of the following statement is correct:

   (a) all d-orbitals are pure

   (b) d_{z^2} orbital is formed by 4 lobes

   (c) all d-orbital's are oriented along axis

   (d) d_{z^2} orbitals form strongest σ bond among all d-orbitals.

8. Which of the following is least diffused directional orbital?
(a) s (b) p (c) d (d) f

9. Select the incorrect geometry for hybridization:
(a) sp = linear (b) sp^3d = T.B.P. (c) sp^3d^2 = P.B.P (d) All are correct

10. Chemical bond implies:
(a) Repulsion (b) Attraction
(c) Attraction and Repulsion (d) None of these

11. Which among the following orbitals have ungerade symmetry?
(a) s-orbital (b) d_{z^2} orbital (c) d_{xy} orbital (d) None of these

12. The overlap between p_y and s orbital along z-axis lead to formation of
(a) σ – bond (b) π – bond
(c) no bond will be formed (d) δ – bond

13. Which of the following orbital cannot form π-as well as δ-bond?
(a) d_{xy} (b) d_{z^2} (c) $d_{x^2-y^2}$ (d) d_{yz}

14. Select the correct statement:
(a) The hybrid orbitals may be equivalent or not.
(b) The hybridization defines a geometry of the molecule.
(c) The hybrid orbital have greater bonding strength compared to pure atomic orbital
(d) The hybrid orbitals have lesser bonding strength compared to the pure atomic orbitals.

15. Which among the following statement(s) is /are correct:
(a) Penetration and shielding are same.
(b) Penetration is presence of outer e^- density in inner e^- density region.
(c) Penetration is polyorbital phenomenon.
(d) Penetration is multielectronic phenomenon.

16. Select the correct statement for non-bonding and anti-bonding orbitals:
(a) Non-bonding orbitals have same energy as the atomic orbitals from which they are formed.
(b) Anti-bonding orbitals have higher energy than the atomic orbitals from which they are formed.
(c) Non-bonding orbitals having higher energy than the atomic orbitals from which they are formed.
(d) Anti-bonding orbitals have lower energy than the atomic orbitals from which they are formed.

17. The statement(s) correct about Li is:
(a) It is polyelectronic specie
(b) Ground state for Li is 2s
(c) Penetration will not be observed
(d) First excited state is triply degenerate.

18. How many among the following orbitals can for π – bond.

p_x, d_{z^2}, $d_{x^2-y^2}$, s, d_{xz}, p_y, p_z

19. Among the following number of orbitals have two nodal planes –

$d_{z^2}, d_{x^2-y^2}, d_{xy}, p_x, s$

××××

QUANTA CHEMISTRY
An Institute of Chemical Sciences

ANSWER KEY

1.	(d)	8.	(b)	15.	(b, c, d)
2.	(b)	9.	(c)	16.	(a, b)
3.	(d)	10.	(b)	17.	(a, b, d)
4.	(d)	11.	(d)	18.	5
5	(b)	12.	(c)	19.	2
6.	(d)	13.	(b)		
7.	(d)	14.	(a, b, c)		

HINTS & SOLUTIONS

1. (d)

Sol. He^+ is monoelectronic specie and subshells of same shell will be degenerate due to absence of penetration and shielding.

2. (b)

Sol.

$He \Rightarrow 2e^-$ $\qquad$ $He^+ \Rightarrow 1e^-$

$\vdots$

3p_____

3s_____ (4^{th} energy level) $\qquad$ $\overline{4s}$ $\overline{4p}$ $\overline{4d}$ $\overline{4f}$ (4^{th} energy level)

2p_____ (3^{rd} energy level) $\qquad$ $\overline{3s}$ $\overline{3p}$ $\overline{3d}$ (3^{rd} energy level)

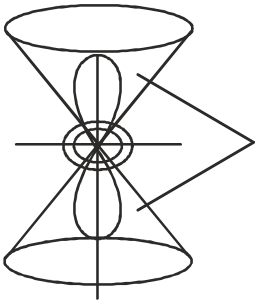
2s_____ (2^{nd} energy level) $\qquad$ $\overline{2p}$ $\overline{2p}$ (2^{nd} energy level)

1s$\underset{\downarrow}{\uparrow}$ (1^{st} enegy level) $\qquad$ $\underset{\downarrow}{\uparrow}$ $\overline{1s}$ (1^{st} energy level)

3s $\Rightarrow$ singly degenerate = 1 $\qquad$ 4s, 4p, 4d, 4f $\Rightarrow$ 1 + 3 + 5 + 7 = 16

Correct option is (b)

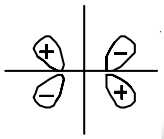
3. (d)

Sol.  two conical nodes

Correct option is (d)

4. (d)

Sol. π^*2p_y orbital



Correct option is (d)

5 (b)

Sol. Since d_{z^2} have 2 bigger lobes and a circular ring while all other d-orbitals have 4 lobes shows differential shielding effect in comparsion to d_{z^2}.

6. (d)

Sol. Non-bonding MO's are formed when symmetry is not matched i.e., orientation of orbitals is not suitable for mixing.

Correct option is (d)

7. (d)

Sol. d_{z^2} is impure d-orbitals

d_{z^2} is formed by 8 lobes

only axial d-orbitals are oriented along axis.

8. (b)

Sol. p-orbital is least diffused directional orbital.

9. (c)

Sol. Pentagonal bipyranidal geometry is sp^3d^3 hybridization, sp^3d^2 is octahedral geometry.

Correct option is (c)

10. (b)

Sol. Any attractive forces between two chemical species forms a chemical bond.

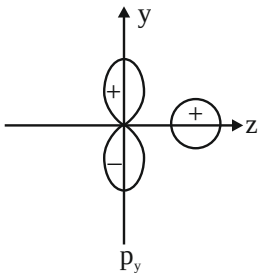
Correct option is (b)

11. d

Sol. All the given orbitals have gerade symmetry i.e. centre of symmetry is present in them.

12. (c)

Sol.



Not in proper orientation for bond formation hence no bond will be formed.

13. (b)

Sol. π-bond invove 2 lobe-2 lobe interaction while δ-bond involve 4 lobe- 4 lobe interaction and none of these are possible in d_{z^2} because circular ring interferes while 2 lobes are interacting with another two and δ-bond is not possible because d_{z^2} donot have 4 lobes.

14. (a, b, c)

Sol. Hybrid orbitals are equivalent only is case of ideal mixing.

Hybridization defines the geometry of the molecule.

Hybrid orbitals have better tendency to form strong bonds.

Correct option is (a), (b) and (c)

15. b, c, d

Sol. Penetration is defined as presence of outer e^- density in inner e^- density region and its is multi electron and polyorbital phenomenon.

16. a, b

Sol. Non-bonding orbitals have same energy to as that of atomic orbital from which they are formed.

ABMO are higher in energy than atomic orbitals.

Correct option are (a) and (b)

17. a, b, d

Sol. $Li \Rightarrow 1s^2 2s^1$

Polyelectronic species

Penetration and shielding will be observed

1^{st} e.s. is triply degenerate

Ground state is 2s for lithium.

18. 5

Sol. π – bond is formed by 2 lobe – 2 lobe interaction. Any orbital having 2 lobes is capable of forming a π – bond along suitable axis of interaction.

19. 2

Sol. $d_{x^2-y^2}$ and d_{xy} have two nodal planes whereas s and d_{z^2} do not have any nodal plane. p-orbitals have one nodal plane.

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 2

1. Which of the following involved forced excitation?
   (a) NH_3 (b) PH_3 (c) CH_4 (d) SF_4
2. Which of the following doesn't exist due to fails in primary condition of excitation.
   (a) PH_3 (b) SH_6 (c) NH_5 (d) XeH_6
3. A square planar complex is formed by hybridization of which atomic orbital.
   (a) s, p_x, p_y, d_{yz} (b) $s, p_x, p_y, d_{x^2-y^2}$ (c) s, p_x, p_y, d_{z^2} (d) s, p_x, p_z, d_{xy}
4. Only iodine forms heptafluoride IF_7, but chlorine and bromine give pentafluoride. The reason for this is:
   (a) Low electron affinity of iodine.
   (b) usual pentagonal bipyramidal structure of IF_7
   (c) That the larger iodine atom can accommodate more number of smaller fluorine atom around it.
   (d) Low chemical reactivity of IF_7.
5. Which of the following molecules does not exist?
   (a) He_2 (b) $H - H^+$ (c) $He - He^+$ (d) Li_z
6. Which of the following halides does not exist?
   (a) PbF_4 (b) $PbCl_4$ (c) PbI_2 (d) PbI_4
7. If Hund's rule is not applicable, the bond order and magnetic behaviour of O_2 molecule is:
   (a) 2, paramagnetic (b) 2, diamagnetic (c) 2.5 paramagnetic (d) 2.5 ferromagnetic
8. Calculate the % P character in orbital occupied by the lone pair in water molecule having $\angle HOH = 104.5$ and $\cos(104.5) = -0.25$
   (a) 80% (b) 20% (c) 70% (d) 75%
9. In which of the following pairs of molecules/ions both the species are not likely to exist.
   (a) H_2^+, He_2^{2-} (b) H_2^-, He_2^{2-} (c) H_2^{2+}, He_2 (d) H_2^-, He_2^{2+}
10. Which of the following exist as covalent crystal in solid state.
    (a) Iodine (b) Silicon (c) Sulphur (d) Phosphorus

11. Stability of species Li_2^- and Li_2^+ increase in the order of _____.
(a) $Li_2 < Li_2^+ < Li_2^-$ (b) $Li_2^- < Li_2^+ < Li_2$ (c) $Li_2 < Li_2^- < Li_2^+$ (d) $Li_2^- < Li_2 < Li_2^-$

12. The number of σ and 'π' bonds present in C_3O_2 are respectively
(a) Four and four (b) Four and two (c) Three and four (d) Three and three

13. The paramagnetic species among the following is _____.
(a) Cu^+ ions (b) Singlet oxygen (c) Mo^{6+} ions (d) Triplet oxygen

14. Which of the following attain the linear structure:
(a) $BeCl_2$ (b) $NCO^{\ominus}$ (c) NO_2 (d) CS_2
Correct option are a, b and d

15. Bond length depends upon
(a) Bond order (b) π-bonding
(c) State of hybridization (d) None of these

16. Select the correct statement:
(a) Vander Waals radii is always larger than the covalent radii
(b) The bond length of a particular bond depends on the state of hybridization of the involved atom.
(c) When s% character increase, the bond length increase.
(d) All the incorrect.

17. Which of the following compound possesses Lewis acid character:
(a) AlF_3 (b) SiF_4 (c) PF_5 (d) BF_3

18. The sum of nodal plane of $\sigma^*_{s\text{-}s}$ antibonding molecular orbital and $\sigma^*_{p\text{-}p}$ bonding molecular orbital.

19. Find the number of pi-bonding molecular orbital from the following set of 'z' is inter nuclear axis ___.
p_z and d_{z^2}, p_x and d_{x^2}, d_{x^2} or d_{y^2}

20. Find the ratio of lone pairs present on Cl atom to sp^2 hybrid orbital in $C_3N_3Cl_3$ molecules.

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	(d)	8.	(c)	15.	(a and c)
2.	(c)	9.	(c)	16.	(a, b)
3.	(b)	10.	(b)	**17**.	(b, c, d)
4.	(c)	11.	(b)	18.	1
5.	(a)	12.	(a)	19.	(2)
6.	(d)	13.	(d)	20.	3
7.	(b)	14.	(a, b, d)		

HINTS & SOLUTIONS

1. (d)

2. (c)

2. Primary condition is availability of vacant orbitals. NH_5 donot exist because it fails in primary condition.

Correct option is (c)

3. (b)

3. Square planer is z-excluded geomertry.

$s + p_x + p_y + d_{x^2-y^2}$

Correct option is (b)

4. (c)

4. Larger iodine atom can acconodate more no. of smaller flourine atom around it.

Correct option is (b)

5. (a)

5. He_2 doesnot exist because bond order is zero.

Correct option is (a)

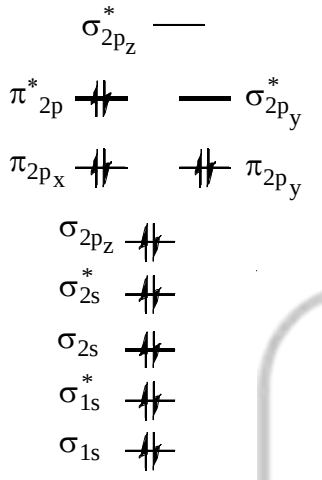
6. (d)

6. PbI_4 doesnot exist.

Correct option is (d)

7. (b)

7. $O_2 : 16e^-$



if Hund's rule is not applicable then,

Bond order = $\frac{10-6}{2} = 2$

Diamagnetic

Correct option is (b)

8. (c)

$\cos\theta = \frac{s}{s-1}$

This s comes out to be 20%.

i.e., 20% of s character is present in each bonds.

% s in lone pair = $\frac{100 - \sum \%s \text{ bonds}}{\text{no. of lone pair}} = 30\%$

% s in each lone pair is 30%

% p in each lone pair = 100 – 30 = 70%.

Correct option is (c)

9. (c)

9. He_2 doesnot exist because its bond order is zero.

Correct option is (c)

10. (b)

10. Silicon exists as : covalent crystal in solid state.

Correct option is (b)

11. (b)

11. In Li_2^+, the electron is to be removed from BMO hence Bond order and stability decreases. In Li_2, the electron is to be added in ABMO, so stability decreases. More the no. of e^- is ABMO, lower is the bond order.

Stability order : $Li_2^{2-} < Li_2^+ < Li_2$

Correct option is (b)

12. (a)

12. C_3O_2

$$O \overset{\sigma}{\underset{\pi}{=}} C \overset{\sigma}{\underset{\pi}{=}} C \overset{\sigma}{\underset{\pi}{=}} C \overset{\sigma}{\underset{\pi}{=}} O$$

four σ and four π bonds

Correct option is (a)

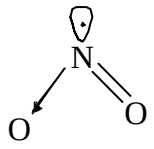
13. (d)

13. Triplet oxygen contain two unpaired electrons hence paramagnetic.

Correct option is (d)

14. (a, b, d)

$Cl-Br-Cl$ (linear) $N\equiv C-O^-$ (linear)

14.  (non-linear) $S=C=S$ (linear)

Correct option are a, b and d

15. (a and c)

15. Bond length $\alpha \dfrac{1}{\text{Bond order}}$

Higher the % s-character, shorter is the bond length.

Higher the % p-character, longer is the bond length.

Correct option are a and c

16. (a, b)

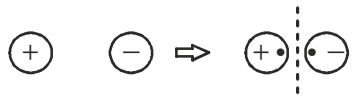
16. Vanderwoal radii > Covalent radii always

Bond length $\propto \dfrac{1}{\%\,s-\text{character}}$

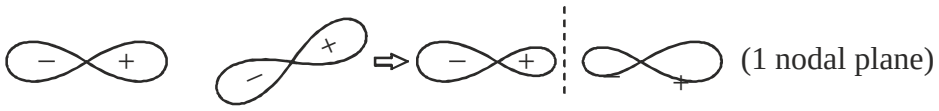
Correct option are a and b

17. (b, c, d)

18. 1


(1 nodal plane)

18.

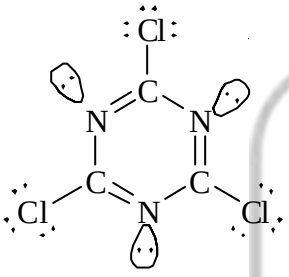

(1 nodal plane)

Correct answer is a, b

19. (2)

20. 3

20.



There are 9 lone pairs of e– present in Sp^2 hybrid orbitals of $C_3N_3Cl_3$

$\therefore$ The ratio = $\frac{9}{3}$.

Correct answer is 3

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 3

1. $(N_5)^+$ cationic species exists in compounds $[N_5^+]$ $[Sb_2F_{11}]$ or in $[N_5]^+$ $[A_5F_6]$. The structure of (N_5^+)

   (a) Linear (b) Angular

   (c) Cyclopentadienyl type (d) Square planar

2. Assuming pure 2s and 2p orbital carbon are used in forming CH_4 molecule, which of the following statement is false?

   (a) Four C – H bond will be at 90°.

   (b) Three C – H bond will be stronger than 4th C – H bond.

   (c) The angle of C – H bond formed by s – s. Overlapping will be uncertain withrespect to other three bonds.

   (d) No. prediction regarding the shape of molecules.

3. Which of the following is a drago compound.

   (a) SiH_4 (b) H_2O (c) PF_3 (d) H_2Te

4. Number of covalent bonds in MgH_2 is:

   (a) zero (b) one (c) two (d) four

5. Which of the following cannot exist on the basis of M.O. theory?

   (a) C_2 (b) He_2^+ (c) H_2^+ (d) He_2

6. The decreasing value of bond angle from NH_3 and SbH_3 down the group –15 of the periodic table is due ____.

   (a) increasing bp – bp repulsion (b) increasing p-orbital character in sp^3

   (c) decreasing lp – bp repulsion (d) increasing electronegativity

7. PCl_5 and PBr_5 exist in sp^3d hybrid state is gaseous phase. But in solid state, when of the following statement is true?

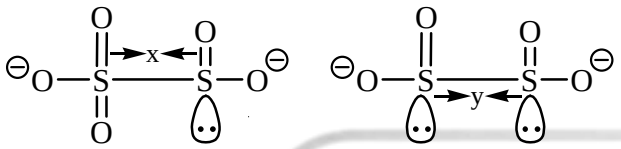
   (a) P is PCl_5 exist in sp^3 while P is pair exist as PBr_5 exist as sp^3d^3 and sp^3 hybridisation.

   (b) P in PCl_5 exist in sp^3d^2 and sp^3 hybridisation. state whole P in PBr_5 exist in sp^3 hybridisation.

   (c) P in PCl_5 exist in sp^3d^2 and sp^3. Hybridisation state while P in PBr_5 exist in sp^3 hybridisation.

   (d) P is PCl_5 and PBr_5 exist in sp^3 hybridisation.

8. If π-back bonding involves the lone pair of central atom, then bond angle gets opened up due to:
   (a) increase in $b_p|b_p$ repulsion for the enhanced bond multiplicity
   (b) decrease in $l_p | l_p$ and $l_p | b_p$ repulsion(s) on central atom.
   (c) Both a and b
   (d) None of these
9. The existence of intermolecular forces is supported by the fact.
   (a) Non ideality of real gases. (b) Liquefaction of gases
   (c) Both a and b (d) None of these
10. Compare S – S bond length from the following molecules:



   (a) x < y (b) y > x (c) x = y (d) None of these
11. If Pauli exclusion principle is not applicable and one orbital has$3e^{\Theta}$, then last e^{Θ} of N_2 molecule is present in
   (a) σ (2s) (b) σ^* (2s) (C) π^* 2py (d) π 2py
12. Assuming 2s–2p mixing is not operative the paramagnetic species among the following is:
   (a) Be_2 (b) Br_2 (C) C_2 (d) N_2
13. Predict the nature of metal oxide is ϕ = 2% for metal cation.
   (a) Amphoteric (b) Acidic (c) Basic (d) Neutral
14. Maximum number of atom that be in same plane in PCl_5 molecules.
   (a) 4 (b) 2 (c) 3 (d) 1
15. Select the correct statement: 1st ionization potential:
   (a) $N_2 > O_2$ (b) $N_2 > O$ (c) $O > O_2$ (d) $O_2 = N_2$
16. Select the correct statement(s)
   (a) e^{Θ} cloud of cation will get deformed by that of the anion, but as the electron in the cation are much more highly bond due to the excess positive change on cation so distortion is negligible.
   (b) With the increase of ionic potential, the polarising power of cation increase and degree of covalency increase.
   (c) With the increase of ionic potential, the polarising power of cation increase.
   (d) With the decrease of ionic potential the polarizing power of cation increase.
17. If x is internuclear axis, then which type of overlapping is/are responsible for the formation of N.B.M.O.?
   (a) $d_{xy} + p_x$ (b) $d_{xy} + s$ (c) $s + p_y$ (d) $s + p_z$
18. In PO_4^{3-} ions the formal charge on oxygen atom of P – O bond is : ____.
19. The number of non-bonding molecular orbital from the following set if 'z' is the internuclear axis ____.

××××

QUANTA CHEMISTRY

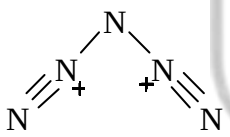
An Institute of Chemical Sciences

ANSWER KEY

1.	(b)	8.	(c)	15.	(a, b, c)
2.	(a)	9.	(c)	16.	(a, b, c)
3.	(d)	10.	(b)	17.	(a, b, c, d)
4.	(a)	11.	(d)	18.	1
5.	(d)	12.	(c)	19.	3
6.	(b)	13.	(c)		
7.	(c)	14.	(a)		

HINTS & SOLUTIONS

1. (b)

1.  (angular)

Correct option is (b)

2. (a)

2. The three p-orbitals forming bonds at 90° while the fourth bond formed by s-orbital won't be forming 90° angle angle because s-orbitals are non-directional.

Correct option is (a)

3. (d)

3. H_2 Te is a drago molecule.

Correct option is (d)

4. (a)

4. There are no covalent bonds is MgH_2 because it is ionic.

Correct option is (a)

5. (d)

5. He_2 doesnot exist because its bond order is zero.

Correct option is (d)

6. (b)

6. The decrease bond angle on going from NH_3 to SbH_3 is due to increasing p-orbital character as the molecules start behaving as drago molecules.

Correct option is (b)

7. (c)

7. PCl_5 is solid state exist as $[PCl_6^-]$ and $[PCl_4]^+$ which are sp^3d^2 and sp^3 hybridized respectivity.

PBr_5 is solid state exist as $[PBr_4^+]$ which is sp^3 hybridized.

Correct option is (c)

8. (c)

8. The bond angle increases because of ↑sed b.p–b.p repulsion as the bond multiplicity is enhanced and there is a decrease in l.p – l.p and l.p – l.p repulsion on central atom.

Correct option is (c)

9. (c)

9. Non-ideality of real gases and liquefaction of gases supports the existance of intermolecular forces.

Correct option is (c)

10. (b)

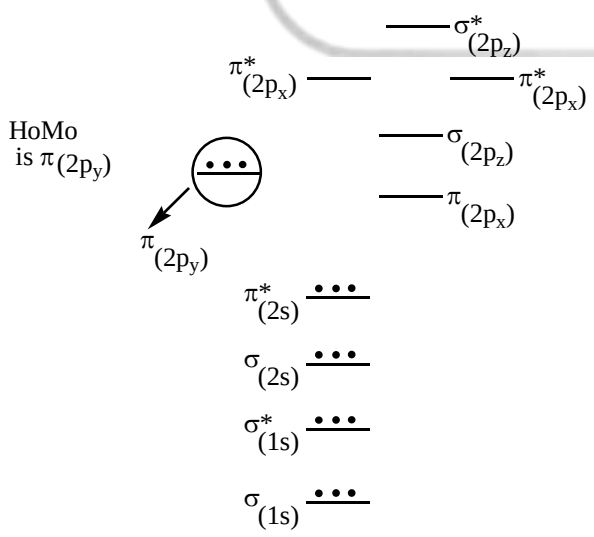
10. L.p are more s-philes than double bond hence required more s-character thereby the S-S bond length increase because reduced %S in this bond.

Correct option is (b)

11. (d)

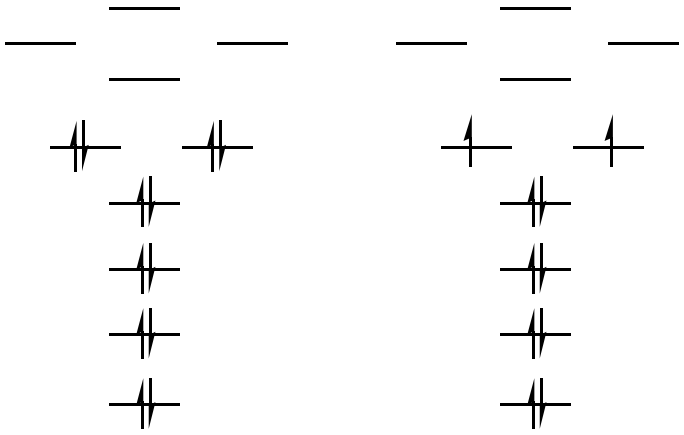
11. If pauli's exclusion principle is not applicable then–

$N_2 \rightarrow 14e^-$



12. (c)

12.



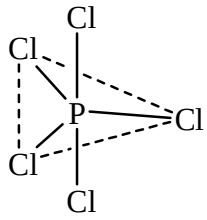
with s-p mixing
$\Rightarrow$ diamagnetic

without s-p mixing
$\Rightarrow$ paramagnetic mixing

13. (c)

14. (a)

14.



$\Rightarrow$ maximum no. of atoms in a plane = 4

15. (a, b, c)

15. Ionization : Boding MO. > atomic orbital > Antibonding MO energy

- In N_2, e^- is to be removed from BMO
- In O_2, e^- is to be removed from ABMO
- In O, e^- is to be removed from atomic orbital.

16. (a, b, c)

16.
- In highly charged cations, e^- are tightly bound to nucleus hence difficult distortion
- $\downarrow$se in ionic potential, the polarizing power of catin $\uparrow$se covalency increase.
- $\downarrow$se in ionic potential, polarizing power of cation $\uparrow$se.

17. (a, b, c, d)

17. $d_{xy} + P_x$, $d_{xy} + s$, $s + P_y$, $s + P_z$ all form NBMO if x is internuclear axis.

18. 1

18. PO_4^{3-} formal change = (Total no. of valence e^-) – no. of non-bonding electrons $-\frac{1}{2}$ (no. of bonding electrons)
Formal Charge on oxygen = 6 – (6) – (1) = –1

19. 3

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 4

1. Which is correct order of strength of bonding or orbital in given at–
   (a) S – S > S – P > P – P (b) S – S < S – P < P – P
   (c) S – P > S – S > P – P (d) S – P > P – P > S – S
2. Which types of bond is formed by overlapping of $d_{xy} - d_{xz}$ orbital if the molecular axis is x-axis ___.
   (a) σ-bond (b) π-bond (c) δ-bond (d) μ-bond
3. If six-lobes of one orbital and six lobes of other orbital are overlap then the resultant bond is—
   (a) σ (b) π- (c) δ (d) ϕ
4. Which has maximum S% among:
   (a) H_2O (b) H_2S (c) H_2Se (d) All of these
5. The hybridization state of 'B' when B form adduct with either is:
   (a) sp (b) sp^2 (c) sp^3 (d) sp^3d
6. The non-equivalence hybrid orbital are found in
   (I) sp^3 (II) sp^3d (III) sp^2d (iv) sp^3d (iv) sp^3d^3
   (a) II, V (b) II, III, IV, V (c) I, II, IV (d) II, III, V
7. The percentage of d-orbital in axial position in sp^3d, trigonal bipyramidal geometry.
   (a) 50% (b) 25% (c) 20% (d) 33%
8. Hybridisation in MnO_4^{Θ} is
   (a) sd^3 (b) sp^3 (c) p^3d (d) dsp^3
9. In which of the following C – H bond has highest 's' character?
   (a) acetylene (b) Ethylene (c) Methane (d) Ch Radical
10. What (% S) character in lone pair of a molecule AB_2 having two lone pair. Given that % s in (AB) bond is 20%.
    (a) 60% (b) 40% (c) 30% (d) 70%
11. What is % P character in lone pair of H_2O if bond angle is 104.50.
    (a) 51% (b) 31% (c) 71% (d) 29%

12. Pick the ideal hybridisation in molecule.

(a) NH_3 (b) CH_3Cl (c) SiH_4 (d) H_2O

13. % S character in the bond & P–Br bond of PBr_3. Bond angle in PBr_3 is 102°.

(a) 20.79% (b) 17.2% (c) 82.7% (d) 1.72%

14. Which of the following compound has least bond angle?

(1) NH_3 (b) H_2O (c) PH_3 (d) PCl_3

15. Assume following structure of N_2O

(I) $\ddot{N}=\ddot{N}=\ddot{O}$ (II) $:\ddot{N}-N\equiv O:$ (III) $:N\equiv N-\ddot{O}:$ (IV) $\ddot{N}=N=\ddot{O}:$

(V) $:N=N=\ddot{O}$ (VI) $:N=N=\ddot{O}:$

which is/are most stable structure:

(a) I & II (b) III only (c) V and IV (d) Only VI

16. Select the correct statement:

(a) More electronegative atom prefer the hybrid orbital of central atom in which the S-character is less.

(b) More electronegative atom prefer the hybrid orbital of the central atom in which the S-character is less.

(c) Lone pair prefers to stay with that hybrid orbital which has less-s-character.

(d) Lone pair prefer to stay with that hybrid orbital which has more s-character.

17. Select the correct statement(s)

(a) For the same change and same size, a pseudo noble gas type of cation with $18e^{\Theta}$ in outermost shell is more polarising than the cation of noble gas type with $8e^{\Theta}$ in outermost shell.

(b) The degree of covalency increase in descending a group in the transition metal ion for a particular ooidation state

(c) Size increase in descending a group in the transition metal ions for a particular oxidation state.

(d) Covalency decrease in descending in a group in the transition metal ion for particular oxidation.

18. Total number of lone-pair of elctron in melamine is ____.

19. Find the sum of nodal plane of π^* d-d anti-bonding molecular orbital and π^* p – d anti-bonding molecular orbital _____.

20. Find out the number of species showing H – C – H > .....

CH_3F, CH_2F_2 , SH_4, $CH_3C \equiv CH$, SH_4

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

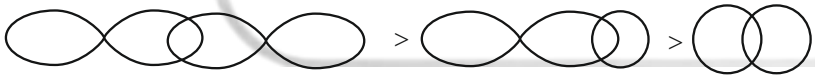
1.	(b)	8.	(c)	15.	(b)
2.	(b)	9.	(a)	16.	(a, d)
3.	(d)	10.	(c)	17.	(a, b)
4.	(c)	11.	(c)	18.	6
5.	(d)	12.	(c)	19.	4
6.	(a)	13.	(b)	20.	4
7.	(a)	14.	(d)		

HINTS & SOLUTIONS

Assignment-04 (Chemical Bonding)

1. (b)

1. bonding strength–



(p – p) (p – s) (s – s)

move is the directional character better is the bonding strength.

2. (b)

2. d_{xy} – d_{xz} will undergo 2 lobe-2lobe interaction hence π-bond formation will take place.

3. (d)

3. 6 lobe - 6 lobe interaction leads to formation of ϕ bond.

4. (c)

5. (d)

5. Boron on formation of adduct leads to formation of sp^3 hybridization.

6. (a)

6. sp^3d and sp^3d^3 are having non-equivalent hybrid orbital.

7. (a)

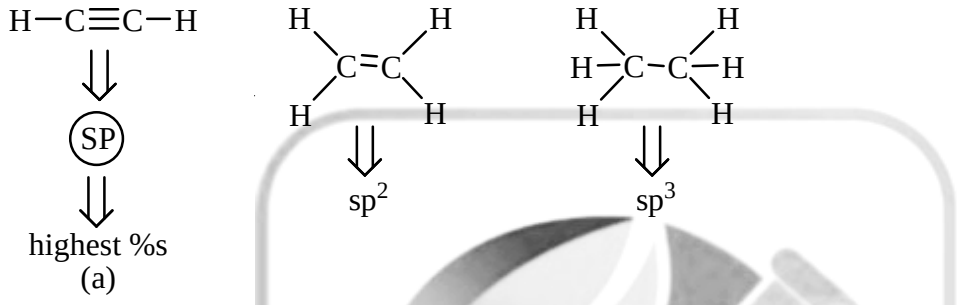
7. In sp^3d hybridization, total orbitals = 5, out of which one is d-orbital

$$\% \text{ d} = \frac{1}{5} \times 100 = 20$$

8. (c)

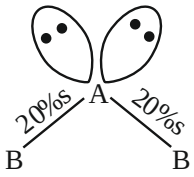
8. MnO_4^- is sd^3 hybridized.

9. (a)

9. 

10. (c)

10. %s in lone-pair = $\dfrac{100 - \Sigma \text{ \%s in bonds}}{\text{Number of lone pair}}$



$$= \frac{100 - 40}{2} = 30$$

%s in each lone pair = 30%

11. (c)

11. $\cos\theta = \dfrac{s}{s-1} \Rightarrow s = 40\%$

%s = 20% in each bond pair.

$$\%\text{s in lone pair} = \frac{100 - \Sigma \text{ \%s in bonds}}{\text{no. of lone pair}} = 30$$

%p in each lone pair = 100 – 30 = 70%

12. (c)

12. SiH_4 do not have any lone pair hence ideal hybridization.

13. (b)

13. $\cos\theta = \frac{s}{s-1}$

$\cos(102°) = \frac{s}{s-1} \Rightarrow -0.207 = \frac{s}{s-1}$

$-0.207s + 0.207 = s$

$s = \frac{0.207}{1.207} = 0.1714$

$\%s = 0.1714 \times 100 = 17.14\% \approx 17.2\%$

14. (d)

14. PH_3 being drago molecule have least bond angle.

15. (b)

15. $N \equiv \overset{+1}{N} - \overset{-1}{O}$

This is the most stable structure of N_2O.

16. (a, d)

16. • More E.N. atom prefers hybrid orbitals with less s-character.

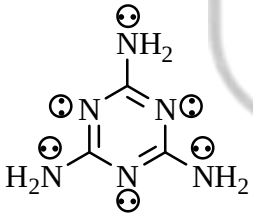
• lone pairs are s-philes hence need mores-character (a & d).

17. (a, b)

17. • harder the charge density on cation, more polarizing will be its nature.

• degree of covalency increases in descending a group in transition metal ion for a particular oxidation state.

18. 6

18. 

6 lone pair of e^- on melamine.

19. 4

20. 4

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CSIR- NET

DPP-(5) CHEMICAL BONDING

1. State of hybridization of Sulphur, Carbon-1 and C_2 in F3SCCF$_3$ respectively

   (a) sp^3, sp^3, sp^3 (b) sp^3 sp^2 sp^3

   (c) sp^3d, sp sp^3 (d) sp^3 sp sp^3

2. Select the correct statement for BrF_5

   (a) All Fluorine atoms are in same plane (b) Four 'F' atoms and 'Br' is in the same plane

   (c) 4 'F' atoms and 'Br' is in the same plane (d) It has at F – Br – F bond angle at 90°

3. Total number of planes which contain 4 atom in a plane are maximum in

   (a) CH_4 (b) PCl_5 (c) XeF_4 (d) SF_4

4. Two isoelectronic pair are formed on matching

(a)	CO, $(CN)_2$	(P)	SO_2, Cyclic $(SO_3)_3$
(b)	$(NH_2)_2CO$, CO_2	(Q)	ICl_2^+, MnO_4^-
(c)	$TeCl_2, CrO_4^{2-}$	(R)	ICl_2^+, MnO_4^-
(d)	$ClO_3^+, Sl_3O_9^{6-}$	(S)	BF, B_2O_3

   According to above statement which of the following option is correct?

   (a) a-(P); b-(Q); c-(R); d-(S) (b) a-(S); b-(Q); c-(R); d-(P)

   (c) A-(S); b-(R); c-(Q); d-(P) (d) a=(P); b-(R); c-(Q); d-(S)

5. In $ICl_2^+, ICl_2^-, ICl_4^-$ sum of bond pair and lone pair on each iodine atom are respectively

   (a) 2, 2 and (b) 2, 3 and 2 (c) 4, 5 and 4 (d) 4, 5 and 6

6. Consider a *p*-orbital of an atom and identify correct statement

   (a) *s*-orbital of another atom produce π bond when Y is bond formation axis

   (b) p_y-orbital of another atom produced σ bond when x is the bond formation axis

   (c) p_2-orbital of another atom produced π-bond when x is bond formation axis

   (d) d_{xy} orbital of another atom pressure π-bond when s is the bond formation axis

7. Which of the following order is correct for dipole moment?

   (a) $CH_3F > CH_3Cl > CH_3Br > CH_3I$

   (b) $CH_3Cl > CH_3Br > CH_3F > CH_3I$

   (c) $CH_3Br > CH_3Cl > CH_3I > CH_3F$

   (d) $CH_3Cl > CH_3F > CH_3Br > CH_3I$

8. Out of given molecules, how many molecules, contain two-pi bonds in between carbon atoms

$CaC_2, C_2Cl_2, C_2HCl, C_2H_2Cl_2, C_2HCl_5$?

(a) Two (b) Three (c) Four (d) Only One

9. In $CuSO_4 \cdot 5H_2O$ total number of H_2O molecule which form coordinate bond with metal is

(a) 2 (b) 4 (c) 5 (d) 0

10. The *d*-orbital which are not involved in hybridization of central atom in ICl_4^-

(a) $d_{z^2}, d_{x^2-y^2}$ (b) $d_{x^2-y^2}, d_{xy}, d_{yz}, d_{zx}$ (c) $d_{x^2}, d_{xy}, d_{yz}, d_{xz}$ (d) d_{xy}, d_{xz}, d_{yz}

11. Which of the following structure of $(CN_2)^2$ is **incorrect**?

(a) $:\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}}^{2}-C\equiv N:$ (b) $-:N=C\equiv \overset{-}{\underset{\cdot\cdot}{N}}:$ (c) $:N\equiv C-\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}}:^{2-}$ (d) $\overset{-}{:}\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}}\equiv C=\overset{\cdot\cdot}{\underset{\cdot\cdot}{N}}:^{-}$

12. Consider the following statements :

(I) Covalency of Hydrogen can't be more than one

(II) Nitrogen can't form more than four covalent bonds

(III) In all the possible non-cyclic Lewis structure of azide in $\left(N_3^-\right)$ central nitrogen has covalency of four

(IV) Maximum covalency of Sulphur is two as it has two unpaired electron in its valance shell

Using T for True and F for False. Correct Answer

(a) F T T F (b) T T T T (c) T F T F (d) T T T F

13. What is the formal charge on carbon in CO and CO_2 respectively?

(a) -1, zero (b) -1, +2 (c) -2, +4 (d) -1, +4

14. $kk\sigma 2s^2\sigma^* 2s^2 \begin{cases} \pi 2p_y^2 \sigma 2p_x^2 \\ \pi 2p_z^2 \end{cases}$ above electronic distribution is observed in

(a) Atomic nitrogen (b) Molecular nitrogen (c) O_2^{2+} ion (d) C_2^{2-} ion

15. Molecule ion in which both the lone pairs are opposite to each other.

(a) XeF_4 (b) SF_2 (c) ClF_3 (d) XeF_5^{Θ}

16. Select correct order of bond energy?

(a) $F_2 > Cl_2 > Br_2 > I_2$ (X – X) (b) $N_2 > N_2H_2 > N_2H_4$ (N – N)

(c) $O_2 > O_3 > H_2O_2$ (O – O) (d) $C_2H_4 > C_2H_4 > C_2H_6$ (C – C)

17. Hybrid orbital of an atom have $(sp^3)^2$, $(sp^3)^1$, $(sp^3)^1$, $(sp^3)^1$ electronic distribution. Select correct statement for molecule which is formed by overlapping of required F-atoms.

(a) Molecule will be non-planar

(b) Molecule will be planar

(c) Molecule have total 10 lone pairs

(d) Bond angle will be less than 10%

18. $\underset{(x)}{PF_3} \xrightarrow[\Delta]{F_2(\text{excess})} \underset{(y)}{PF_5} \xrightarrow{F^{\Theta}} \underset{(z)}{PF_5^{\Theta}}$

Find the sum of vacant orbital in the valance shell of phosphorous in (x) and (z) species of above reaction.

19. Number of lone pair-bond pair repulsion at 90 are (P) in I_3^{Θ} .

Number of lone pair-bond pair repulsion at 90° are (Q) in PCl_4^-. Find difference of (P – Q) _____ .0

20. Select number of species which have pyramidal type of structures with square base.

NF_3, SOF_2, IF_5, IOF_4, IO_3^-, XeF_5^-, XeF_5^+, XeO_3

•••••

Answer Key

1.(d) 2.(c) 3.(b) 4.(c) 5.(b) 6.(d) 7.(d) 8.(b) 9.(b) 10.(d) 11.(d) 12.(d) 13.(a) 14.(b,d) 15. (a,d) 16.(b,c,d) 17. (a,b,c,d) 18.(7) 19.(2) 20. (3)

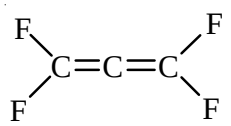
QUANTA CHEMISTRY

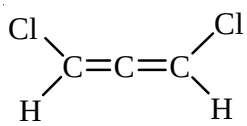
An Institute of Chemical Sciences

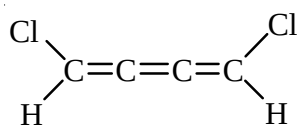
CHEMICAL BONDING

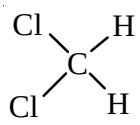
DPP- 6

1. Which molecular geometry is not likely to result, from an octahedral electron geometry.
   (a) Square plannar (b) Pyramidal (c) Linear (d) V-shaped
2. Which of the following is S-phile:
   (a) –F (b) $-CF_3$ (c) $= CF_2$ (d) –Cl
3. Which of the following is not an electron-deficient compound?
   (a) $BeEt_2$ (b) $AlMe_3$ (c) H_6H_6 (d) $Si(CH_3)_4$
4. Which of the following has a zero dipole moment?
   (a) ClF (b) PCl_3 (c) SiF_4 (d) $CFCl_3$
5. The correct order of a dipole moment is:
   (a) $CH_4 > NF_3 < NH_3 < H_2O$ (b) $NF_3 < CH_4 < NH_3 < H_2O$
   (c) $NH_3 < NF_3 < CH_4 < H_2O$ (d) $H_2O < NH_3 < NF_3 < CH_4$
6. Arrange the following compounds in order of increasing dipole moment:
   (I) Toluene (II) M-dichlrobenzene (III) O-dichlrobenzene
   (IV) P-dichlrobenzene
   (a) I< IV< II< III (b) IV < I < II < III (c) IV < I < III < II (d) IV < II < I < III
7. Pauling's electronegativity value of elements are useful in predicting
   (a) Polarity of bonds in molecular (b) Position of elements in periodic table.
   (c) Coordination number (d) Dipole moment of various molecules.
8. Which of the following molecule is polar as well as planar?

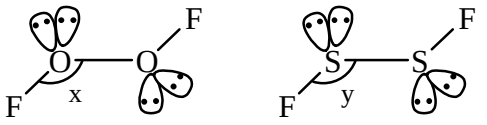
(a) 

(b) 

(c) 

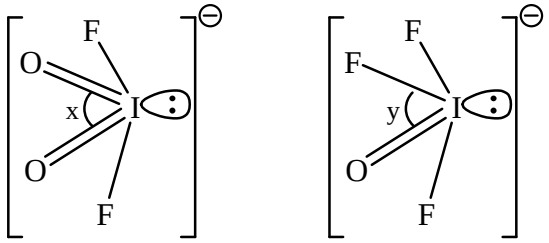
(d) 

9. Compare bond angle for the following molecule:



(a) x > y (b) y > x (c) x = y (d) None of these

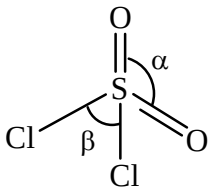
10.



Compare x and y bond angle for the above given molecules

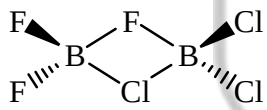
(a) x > y (b) y > x (c) x = y (d) None of these

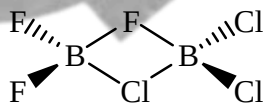
11. Compare α and β bond angle in the following molecule.



(a) α > β (b) β > α (c) α = β (d) None of these

12. What will be the transition state to get BF_2Cl and BCl_2F from the reaction between BF_3 and BCl_3?

(a) 

(b) 

(c) Both a and b (d) None of these

13. Among the following compounds the one that is polar and has the central atom with sp^2-hybridization is

(a) $HClO_2$ (b) BF_3 (c) H_2CO_5 (d) SiF_4

14. Which of the following statement(s) is/are correct?

(a) Dipole moment of Diborane's zero. (b) Diborane is a lewis acid

(c) Diborane has incomplete octet (d) Diborane has 4 2c 2e- bond

15. Select the correct statement(s):

(a) para dihydroxy benzene is polar while para di-methyl benzene is non polar.

(b) Dipole moment of NH_3 is larger than that of NF_3.

(c) The direction of dipole moment in CO is from C to oxygen.

(d) All are incorrect.

16. Select the correct statement(s):

(a) When $d_{x^2-y^2}$ or d_{xy} orbitals combine in parallel planes, then δ or δ^* molecular orbitals are formed.

(b) When $d_{x^2-y^2}$ or d_{xy} orbitals combine in parallel planes, then N.B.M.O. are formed.

(c) When d_{y^2} and d_{x^2} orbitals combine in along the y-axis then N.B.M.O. orbital are formed.

(d) No interaction is possible when P_2 and d_{x^2} orbitals overlap with collinear z-axis.

17. Which of the following species do not exist?

(a) XeF_3 (b) XeF_4 (c) XeF_5 (d) XeF_6

18. Predict the basicity of final product (having sulphur) obtain when SF_4 undergo hydrolysis _____.

19. If Hund's rule is not applicable, then how many unpaired electron are present in NO molecule?

20. Find the number of molecules is/are having zero dipole moment and linear shape from the following

ClF_3, I_3^-, CO_2, $HgCl_2$, ICl_2^-, XeF_2, _____.

××××

QUANTA CHEMISTRY
An Institute of Chemical Sciences

ANSWER KEY

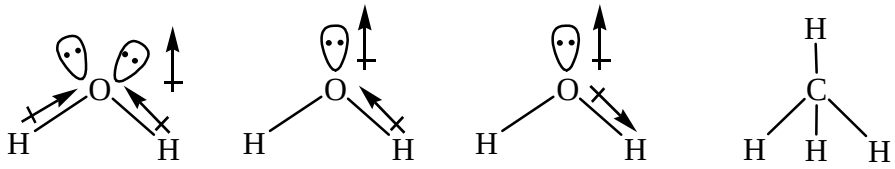
1.	(a)	8.	(b)	15.	(a, b)
2.	(c)	9.	(a)	16.	(a, b, c, d)
3.	(d)	10.	(a)	17.	(a, b, c and d)
4.	(c)	11.	(a)	18.	2
5.	(a)	12.	(a)	20.	5
6.	(b)	13.	(c)		
7.	(d)	14.	(a, b, c, d)		

HINTS & SOLUTIONS

1. (a)
2. (c)
2. Double bonds are s-philes.
   = CF_2 is s-phile
3. (d)
3. $Si(CH_3)_4$ is an e^- precise molecule having its octet complete.
4. (c)

Sol. SiF_4 being ideally tetrahedral have zero dipole moment.

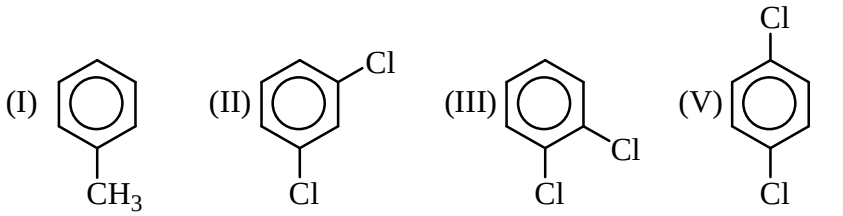
5. (a)

Sol. 

CH_4 being ideal tetrahedal have zero dipole moment.

6. (b)

Sol.



μ = 1.72D μ = 2.54D μ = 0 D

order of dipole moment: III > II > I > IV

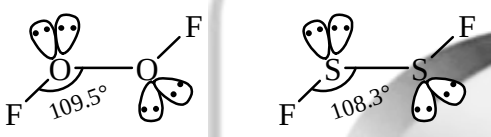
7. (d)

Sol. Pauling's electronegativity value of elements are useful in predicting dipole moment of various molecules.

8. (b)

9. (a)

Sol.



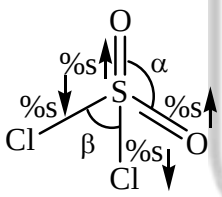
Bond angle in O_2F_2 > S_2F_2

10. (a)

Sol. Double bond are s-philes while flourine is non s-phile and %s α bond angle.

11. (a)

Sol.

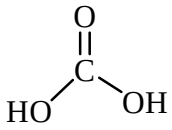


12. (a)

13. (c)

Sol. $HClO_2 \Rightarrow sp^3$ $BF_2 \Rightarrow sp^2$ (non-polar) $H_2CO_3 \Rightarrow sp^2$ (polar)

$SiF_4 \Rightarrow sp^3$ (non-polar)

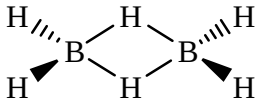


14. (a, b, c, d)

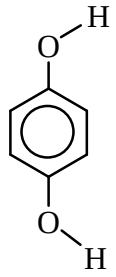
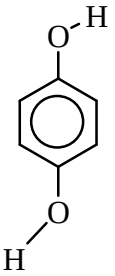
Sol. diborane is B_2H_6

- it has zero dipole moment.
- being e^- deficient can act as lewis acid

• has incomplete octet.

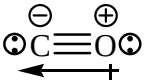
•  $\Rightarrow$ 4 2c - 2e$^-$ bond

15. (a, b)

Sol.  but 

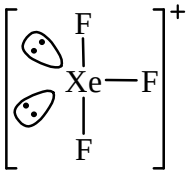
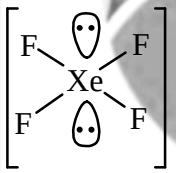
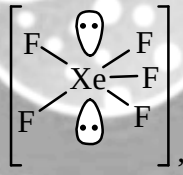
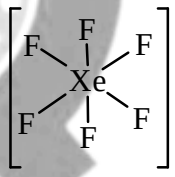
μ = 2.26D μ = 0 D

• $\mu_{NH_3} > \mu_{NF_3}$

• 

16. (a, b, c, d)

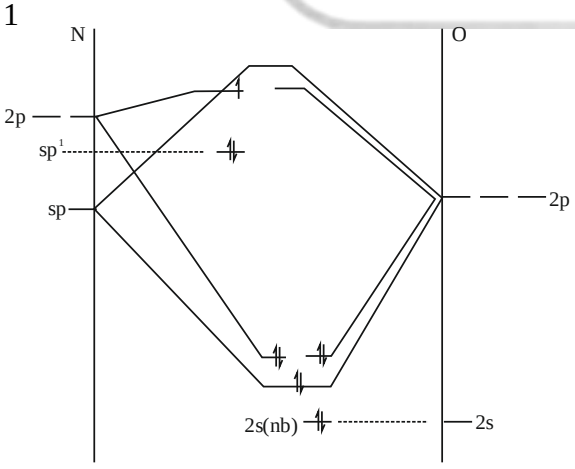
17. (a, b, c and d)

Sol.  ,  ,  , 

all of these exist.

18. 2

19. 1

Sol. 

NO $\Rightarrow$ 11e$^-$

Number of unpaired e^- = 1

20. 5

Sol. $I_3^{\ominus} \Rightarrow$ linear and $\mu = 0$

$CO_2 \Rightarrow$ linear and $\mu = 0$

$XeF_2 \Rightarrow$ linear and $\mu = 0$

$ICl_2^- \Rightarrow$ linear and $\mu = 0$

$HgCl_2 \Rightarrow$ linear and $\mu = 0$

$\therefore$ 5 molecules are linear and have zero dipole moment.

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 7

1. A molecule of type AX_2Ln (L → lone pair n → number) there exist a bond between A and X. LXAY bond angle ____.

   (a) Always decrease if n increase
   (b) Always increase if n increase
   (c) will be maximum for n = 3.0
   (d) Generally decrease if n decrease.

2. Halogen form compound among themselves with the formula XX′, XX & XX'_7 (where X′ is the heavier halogen) which of the following pair represent correct geometry with polar and non-polar nature.

   (a) XX'_3 – linear – polar
   (b) XX – linear – polar
   (c) XX′ – linear – non-polar
   (d) XX'_7 – pentagonal bipyramidal nonpolar

3. Match the following:

Column I	Column II
(a) XoF_4^+	(P) Sec-saw
(b) $Xo_2F_2^-$	(Q) Trigonal bipyramidal
(c) XeO_6^{4-}	(R) Linear
(d) XeF_2	(S) Square planar

   (a) (a – Q), (b – P), (c – S) (d – R)
   (b) (a – P), (b – Q), (c – S) (d – R)
   (c) (a – Q), (b – P), (c – R) (d – S)
   (d) (a – Q), (b – Q), (c – P) (d – R)

4. Which of the following is an example of a non-planar molecule (or ion)?

   (a) Carbonate
   (b) Perchlorate
   (c) Xenon-tetrafluoride
   (d) boron-trifluoride

5. Which of the two following molecules/ions have planar structure?

   (i) XeF_4 (b) ClO_4^- (iii) $PtCl_4^{2-}$ (iv) MnO_4^-

   (a) i and iii
   (b) i and ii
   (c) ii and iii
   (d) ii and iv

6. Three examples of molecules/ions having linear geometry may be given *****.

   (a) CO_2, NCS^- and NO_2^+
   (b) CO_2 $NCS^{\ominus}$ and NO_2
   (c) NO_2, $N_2^{\ominus}$ and $NCs^{\ominus}$
   (d) ClO_2, CO_2 and NO_2^+

7. Match list-I (Compounds) with list-II (Structure) and select the correct answer using the codes given below:

List-I	List-II
(A) XeO_4	(i) Square planar
(B) BrF_4^-	(ii) Tetrahedral
(C) $SeCl_4$	(iii) distorted tetrahedral

(a) (A-ii) (B-iii) (C-i) (b) (A-iii) (B-i) (C-ii)

(c) (A-ii) (B-i) (C-iii) (d) (A-i) (B-ii) (C-iii)

8. In SiF_6^{2-} and $SiCl_6^{2-}$, which one is know and why?

(a) SiF_6^{2-} because of small size of F (b) $SiCl_6^{2-}$ because of large size of F

(c) $SiCl_6^{2-}$ because of small size of Cl (d) $SiCl_6^{2-}$ because of large size of of Cl

9. In which of the following sets do we have sp^3d hybridisation?

(a) XeF_2, IBr_3, XeO_3 (b) IBr_3, SF_5^+, SF_5^- (c) XeF_2, IBr_3, SF_5^+ (d) SF_5^+ and SF_5^-

10. Which of the following species/molecules have same shape but different hybridization?

(a) XeF_2. CO_2 (b) I_3^-, $HgCl_2$ (c) $OCl^{\ominus}$, CO (d) SO_2, OCl_2

11. Identify the interhalogen compound with zero dipole moment.

(a) ICl_3 (b) BrF_5 (c) IF_7 (d) IF_5

12. Which of the following interhalogens cannot exist?

(a) ClF_5 (b) ClI_5 (c) ICl_2^- (d) $IF_4^{\ominus}$

14. Select the correct statement for thiazyl trifluoride (NSF_3)

(a) S – N bond length is 141.5 Pm probably shortest one between S and N.

(b) The three highly electronegative fluorine substituent contract the 3d-orbitals of sulphur sufficiently to effect the strong A-bonding with the half-filled p-orbital of nitrogen

(c) The bond angle F – S – F = 94°. Indicate the involvement of almost prep-orbitals of S in binding the fluorine atoms.

(d) Thus very strong bonding (due to multiple bond formation) between N and S demands the participation of S-character enriched orbitals of sulphur.

15. Correct statement(s) about NH_3 and PH_3 is/are:

(a) μD of PH_3 < μD of NH_3 (b) PH_3 is stronger lewis base than NH_3

(c) $\angle H - N - H > \angle H - P - H$ (d) Both have sp^3 hybridisation

16. Select the correct properties for the following molecules:

(i) CH_2F_2 (ii) CHF_3 (iii) CH_3F

(a) C – F bond length order: $CH_3F > CH_2F_2 > CHF_3$.

(b) C – H bond length order : $CH_2F > CH_2F_2 > CHF_3$.

(c) Shape is not perfect tetrahedral for given compound.

(d) Dipole moment is non-zero for given compound.

17. Correct order of bond energy for PH_3, NH_3 and NF_3, PF_3

(a) $B.D.E_{N-H} > B.D.E_{P-H}$ (b) $B.D.E_{N-H} < B.D.E_{P-H}$

(c) $B.D.E_{N-F} > B.D.E_{P-F}$ (d) $B.D.E_{N-F} < B.D.E_{P-F}$

18. Based on VSEPR theory, the number of 90° F – Br – F angle in a molecule of BrF_5 is _____.

19. Among the following, the number of compound that can react with PCl_5 to give $POCl_3$ is ____.
O_2, CO_2, SO_2, H_2O, H_2SO_4, P_4O_{10}

20. A list of species having the formula SZ_4 is given below:
XeF_4, SF_4, SiF_4, BF_4^-, $[Cu(NH_3)_4]^{2+}$, $[FeCl_4]^{2-}$ and $[CoCl_4]^{2-}$
Defining shape on the basis of the location of 'X' and 'Z' atoms, the total number of species having a square planar shape is:

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	(c)	8.	(a)	16.	(a, b, c, d)
2.	(a)	9.	(c)	18.	zero
3.	(a)	10.	(b, c, d)	19.	5
4.	(b)	11.	(c)	20.	2
5.	(a)	12.	(b)		
6.	(a)	14.	(a, b, c, d)		
7.	(c)	15.	(a, c)		

HINTS & SOLUTIONS

1. (c)

Sol. AX_3L_n

if n = 3

Bond angle is maximum if n = 3 because bond angle is 180° (highest)

Correct option is (c)

2. (a)

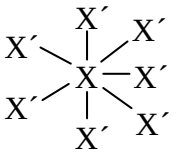
Sol. $XX'_3 \Rightarrow$ non – linear

$XX \Rightarrow$ linear, non –polar

$XX' \Rightarrow$ linear, polar

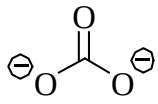
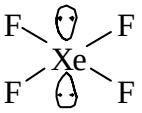
$XX'_7 \Rightarrow$ pentagonal bipyramidal

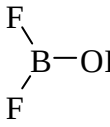
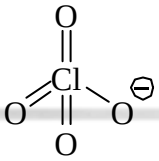
It is non planar because dipole moment around each bond gets cancel out.



3. (a)

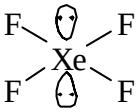
4. (b)

Sol.  (planar)  (square planar)

 (planar)  (non-planar)

Correct option is (b)

5. (a)

Sol.  (square planar)

ClO_4^- and $MnO_4^- \Rightarrow$ tetrahedral

Correct option is (a)

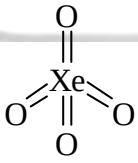
6. (a)

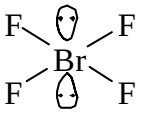
Sol. O = C = O $[N = C = S]^-$ $[O \leftarrow N^+ = O]$

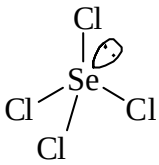
All these molecules are linear

Correct option is (a)

7. (c)

Sol. $XeO_4 \Rightarrow$  $\Rightarrow$ tetrahedral

$BrF_r^{\Theta} \Rightarrow$  $\Rightarrow$ Square planar

$SeCl_4 \Rightarrow$  $\Rightarrow$ distorted tetrahedal

Correct option is (c)

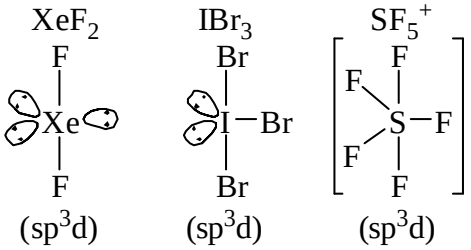
8. (a)

Sol. SiF_6^{2-} is know because F being smaller in size and more E.N. gives favourable conditions for existing while Cl being larger in size will be sterically unstable.

Correct option is (a)

9. (c)

Sol. sp^3d is observed in TBP and square pyramidal



Correct option is (c)

10. (b, c, d)

Sol. I_3^- is linear and sp^3d hybridized and $HgCl_2$ is also linear but sp hybridized.

$OCl^{\ominus}$ is linear but (tetrahedral geometry) sp^3 hybridized and CO is sp hybridized linear.

SO_2 is sp^2 hybridized and bent while OCl_2 is sp^3 and bent.

Correct option are (b, c, d)

11. (c)

Sol. IF_7 have PBP geometry in which dipole moment of each bond is cancelled by the other bond present opposite to that.

Correct option is (c)

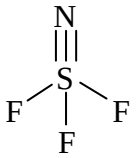
12. (b)

Sol. ClI_5 cannot exist because for existance of of interhalogens, side atoms should be more electronegative than central atom.

Correct option is (b)

14. (a, b, c, d)

Sol. There is a triple bond between S and N



all the given statements are correct

Correct option are (a, b, c, d)

15. (a, c)

Sol. NH_3 is more polar than PH_3

NH_3 is sp^3 hybridized while PH_3 is drago.

$\therefore \angle NH_3 > \angle PH_3$

Correct option are (a, c)

16. (a, b, c, d)

Sol. Bond length $\propto \frac{1}{\%\,s-\text{character}}$

F being more E.N, requires less % s-character.

Correct option are (a, b, c, d)

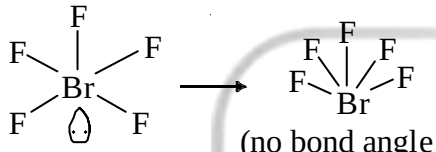
17. (a, d)

Sol. NH_3 being sp^3 hybridized from better bond than PH_3 (drago molecule)

P – F bond being more polar have more ionic character hence stronger than N – F bond.

(a, d)

18. zero

Sol. 

(no bond angle is BrF_5 is of 90^o)

Correct answer is zero

19. 5

20. 2

Sol. XeF_4, $[Cu(NH_3)_4]^{2+}$ are square planar.

Correct answer is 2.

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP-8

1. O_2F_2 is cm unstable yellow orange solid and H_2O_2 is a colorless liquid both have O–O bond O–O bond length in H_2O_2 and F_2O_2 is respectively

   (a) 1.22Å, 1.48Å (b) 1.48Å, 1.22Å (c) 1.22Å, 1.22Å (d) 1.48Å, 1.48Å

2. Which of the following molecules do not have open book structure

   (a) O_2F_2 (b) H_2O_2 (c) S_2Cl_2 (d) H_2C_2

3. According to VSEPR theory, the geometry with lone pair around the central iodine in I_3^+ and $I_3^\ominus$ ions respectively are

   (a) Tetrahedral and Tetrahedral (b) Trigonal bipyramidal and T.B.P

   (c) Tetrahedral and T.B.P. (d) Tetrahedral and Octahedral

4. The Xenone compound that are isostructural with IBr_2 and BrO_3^- respectively are

   (a) Linear XeF_2 and pyramidal XeO_3 (b) Bent XeF_2 and pyramidal XeO_3

   (c) Bent XeF_2 and planar XeO_3 (d) Linear XeF_2 and tetrahedral XeO_3

5. The Geometries of $[Br_3]^+$ and $(I_5)^+$ respectively are

   (a) Trigonal and Tetrahedral (b) Tetrahedral and Trigonal bipyramidal

   (c) Tetrahedral and Tetrahedral (d) Linear and trigonal pyramidal

6. The structure of XeF_2 and XeO_2F_2 respectively are

   (a) bent, tetrahedral (b) linear, square, planar

   (c) linear, see saw (d) bent, see saw

7. Match the following :

	Hybridization		Atomic Orbital
A.	d^2sp^3	(i)	$d_{x^2+y^2}+s+p_x+p_y$
B.	d_{sp^3} TBP	(ii)	$d_{z^2}+s+p$
C.	d_{sp^3} sp	(iii)	$d_{x^2-y^2}+s+d_{z^2}+p$
D.	d_{sp^2}	(iv)	$d_{x^2+y^2}+s+d_{z^2}+p$

   (a) A-(i); B-(iv) ; C-(ii) ; D-(iii) (b) A-(iv); B-(ii); C-(iii); D-(i)

   (c) A-(iv) ; B-(iii) ; C –(ii) ; D-(i) (d) A-(i); B-(ii); C-(iii) ; D-(iv)

8. Overlapping of the following combination of orbital (Assuming Z is integer nuclear axis)

   P : $p_2 + dxy$ R : $s + dyz$ Q : $s + dz^2$

   Comment on native of molecular orbital formed

   (a) P and Q no net overlapping (b) P, R no net overlapping and Q form σ Bond

   (c) R, Q form σ bond and P no net overlapping (d) P, Q, R no net overlapping

9. Among $SiCl_4$, $POCl_3$, NF_3 *trans* $\left[SnCl_4(py)_2\right]$ those with zero dipole moment are

   (a) $SiCl_4$ and NF_3 (b) $SiCl_4$, $POCl_3$ and trans $\left[SnCl_4(py)_2\right]$

   (c) $SiCl_4$, trans $SnCl_4(py)_2$ (d) NF_3 and $SnCl_4(py)_2$

10.

	Hybridization		Atomic Orbital
A.	$FeXO(OSO_2F)$	(i)	Linear
B.	$FXeN(SO_2F)_2$	(ii)	Pyramidal
C.	XeO_3	(iii)	T-shaped
D.	$XeOF_2$	(iv)	Bent

   (a) A-(i); B-(i) ; C-(ii) ; D-(iii) (b) A-(i); B-(i); C-(ii); D-(iv)

   (c) A-(iv) ; B-(i) ; C –(ii) ; D-(iii) (d) A-(i); B-(iv); C-(ii) ; D-(iii)

11. The compound with planar Geometry is

   (a) $N(t\text{-}Bu)_3$ (b) NPh_3 (c) NF_3 (d) $N(Sin_3)_3$

12. Molecules having non-polar as well as polar bonds but the molecules as a whole in planar

   (a) S_2F_2 (b) N_2O_4 (c) Si_2H_6 (d) I_2Cl_6

13. Both $N(SiH_3)_3$ and $NH(SiH_3)_2$ compound have trigonal planar skeleton. Incorrect statement about both compound is

   (a) Si-N-Si bond angle in $N(SiH_3)_3$ > Si-N-Si bond angle in $N(SiH_3)_3$

   (b) N-Si bond length in $NH(SiH_3)_2$ > N-Si bond length in $N(SiH_3)_3$

   (c) N-Si bond length in $NH(SiH_3)_2$ < N-Si bond length in $N(SiN_3)_3$

   (d) Back bonding strength in $NH(SiH_3)_2$ >back bonding strength in $N(SiH_2)_3$

14. Which of the following sets of molecule(s) is/are having a V-shape but different hybridization?

   (a) $SnCl_2$ and H_2O (b) SO_2 and NO_2^+ (c) BF_2^- and SCl_2 (d) OF_2 and SCl_2

15. Which of the following statement(s) is/are correct?

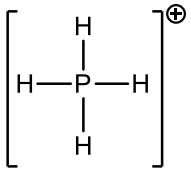
   (a) Every Abs molecules does in fact have a square pyramidal structure

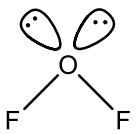
   (b) Multiple bond are always shorter than corresponding single bond

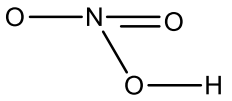
   (c) The electron-deficient molecules can act as Lewis acid,

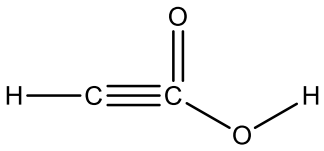
   (d) A sigma bond is formed by side-wise-side overlapping

16. Which of the following correctly represent the bonding capacity of the atom involved

   (a) 

   (b) 

(c) 

(d) 

17. How many molecules are planar from the following molecules _____ .

$I_3^-, H_2O, ICl_2^-, C_2H_4, C_2H_2, H_3O^+$

18. How many molecules have same type of shape from the following molecules?

$H_3O^+, NH_3, ClO_3^+, Ph_3, H_2O, \overset{\ominus}{C}H_3$ _____ .

•••••

Answer Key

1.(b) 2.(d) 3.(c) 4.(a) 5.(b) 6.(c) 7.(b) 8.(b) 9.(c) 10.(a) 11.(d) 12.(a) 13.(b) 14.(a,c) 15. (b,c) 16.(a,b,c,) 17. (5) 18.(4)

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 9

1. The geometry around the central atom in ClF_4^+ is:
   (a) square planar (b) square pyramidal
   (c) Octahedral (d) Trigonal bipyramidal
2. The shape of molecules XeO_2F_2 is:
   (a) Distorted tetrahedral (b) Square planar
   (c) Trigonal bipyramidal (d) Square bipyramidal
3. The bond angle of Cl_2O is:
   (a) Smaller than of F_2O (b) Greater than that of H_2O
   (c) Smaller than that of H_2O (d) Same as that of F_2O
4. Icosahedral structure is generally exhibited by:
   (a) C (b) Sf (c) Ge (d) B
5. If the dipole moment of HCl is 1.08 D and bond distance 1 × 1.27 Å, the partial change on hydrogen and chlorine respectively are:
   (a) + 1, – 1 (b) + 0.85, – 0.85 (c) + 0.36, – 0.36 (d) + 0.178, – 0.178
6. The structure of $N(CH_3)_3$ and $N(SiH_3)_3$ respectively:
   (a) Trigonal planar and pyramidal (b) Pyramidal and trigonal planar
   (c) Pyramidal and pyramidal (d) Trigonal planar and trigonal planar
7. The xenon compounds that are isostructural with IBr_2^- and $BrO_3^\ominus$ respectively are:
   (a) Linear XeF_2 and pyramidal XeO_3 (b) Bent XeF_2 and pyramidal XeO_3
   (c) Bent XeF_2 and planar XeO_3 (d) Linear XeF_2 and tetrahedral XeO_3
8. The structure of O_3 and $N_3^\ominus$ are :
   (a) Linear and bent respectively (b) Both linear
   (c) Both bent (d) Bent and linear respectively
9. The covalency of nitrogen in HNO_3 is:
   (a) 0 (b) 3 (c) 4 (d) 5

10. Which of the following has been arranged in increasing order of size of the hybrid orbitals.
(a) sp, sp^2, sp^3 (b) sp^3, sp^2. sp (c) sp^2, sp, sp^3 (d) sp, sp^3, sp^2

11. S1 : $[XeF_7]^+$ has sp^3d^3 hybridisation S2 : $[PtCl_4]^+$ has sp^3d^3 hybridization
S3 : $[SF_6]$ has sp^3d^3 hybridisation S4 : $[PF_4]^+$ non sp^3 hybridization
(a) TFFT (b) TTFT (c) TFTT (d) FFFT

12. In which of the following pair hybridization of the control atom are different:
(a) ClF_3, ClF_3O (b) ClF_3O, ClF_3O_2
(c) $[ClF_2O]$ $[ClF_4O]^-$ (d) $[ClF_4O]$ $[XeOF_4]$

13. Which of the following statement is true for $IO_2F_2^-$?
(a) The electrons are located at the croners of a trigonal bipyramidal but one of the equatorial pair is unsaturated.
(b) It has sp^3d hybridization and it is T-shaped.
(c) Its structure is analogous to SF_4.
(d) (a) and (c) both.

14. In which of the following molecules number of lone pair and bond pair on central atom are not equal?
(a) H_2O (b) $Ze^{\ominus}$ (c) O_2F_2 (d) SCl_2

15. The bond strength increase:
(a) with increasing bond order
(b) with increasing extent of overlapping of orbital
(c) with decreasing difference between energy of overlapping orbital.
(d) with decrease bond order

16. Which of the following molecules is/are non-planar as well as non-polar?
(a) SF_4 (b) XeF_4 (c) CCl_4 (d) NF_4^+

17. The dipole moment of AX_3, YX_3 and ZW_3 are 4.97×10^{-30}, 0.60×10^{-30} and zero can respecetively select the correct statement(s)
(a) Both AX_3 and YX_3 are planar
(b) Both AX_3 and YX_3 are pyramidal
(c) ZW_3 is pyramidal
(d) ZW_3 is planar

18. How many minimum atoms lie in same plane in $FC_2 = C = CF_2$ molecule_____.

19. Find the number of molecule(s) / ions having lewis basic properties from the following:
H_2O, NH_3, CH_3NH_3, ROH, $FeCl_3$, SO_3.

20. Find the number of molecule(s) / ions having lewis acidic properties from the following:
H_2O, NH_3, H^+, BF_3, AlH_3, Cu^{2+}, $CH_3^{\ominus}$

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

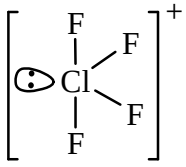
ANSWER KEY

1.	d
2.	c
3.	b
4.	d
5.	d
6.	b
7.	a
8.	d
9.	c
10.	a
11.	c
12.	c
13.	d
14.	b
15.	a, b, c
16.	c, d
17.	b, d
18.	5
19.	4
20.	4

HINTS & SOLUTIONS

1. d

Sol. ClF_4^+

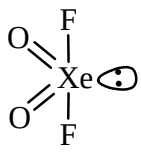


TBP geometry

Correct answer is (d).

2. c

Sol. XeO_2F_2



$\Rightarrow$ TBP geometry and see-saw shape.

Correct answer is (c).

3. b

Sol. Bond angle of Cl_2O is greater than both H_2O and F_2O because NBEPR dominates in case of Cl_2O.

Correct answer is (b).

4. d

5. d

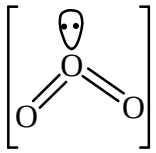
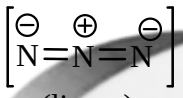
6. b

Sol. In case of $N(CH_3)_3$, there is no backbonding observed hence its shape is pyramidal while in $N(SiH_3)$, due to backbonding it becomes trigonal planar.

Correct answer is (b).

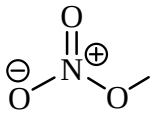
7. a

8. d

Sol. $O_3 \rightarrow$  (Bent) and N_3^-  (linear)

Correct answer is (d).

9. c

Sol.  $\Rightarrow$ Nitrogen has formed 4 bonds in HNO_3.

Covalency is the number of bonds formed by the central atom.

Correct answer is (c).

10. a

Sol. Size of orbital α directional character

more the % p-character in a hybrid orbital, more will be the size.

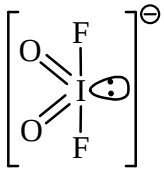
order of size: $sp < sp^2 < sp^3$

Correct answer is (a).

11. c

12. c

13. d

Sol. 

• it has TBP geometry and see-saw shape.

• one equitorial pair is unsaturated.

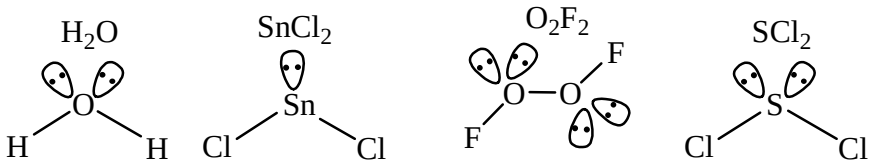
• the hybridization is sp^3d

• its structure is analogous to SF_4

Correct answer is (d).

14. b

Sol.



no. of lone pair on central atom	2	1	2	2
no. of bond pair on central atom	2	2	2	2

Correct answer is (b).

15. a, b, c

Sol. • Bond strength α bond order

• Bond strength α extent of overlapping.

• Lower the difference between overlapping orbitals, lower will be extent of overlap hence lower bond strength.

Correct answer is (a), (b) and (c).

16. c, d

Sol. • SF_4 is non-planer but polar

• CCl_4 is non-planer as well as non-polar

• NF_4^{+9} is non-planer as well as non-polar

• XeF_4 is planer and non-polar

Correct answer (c) and (d)

17. b, d

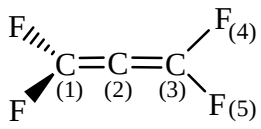
Sol. AX_3 and $YX_3 \rightarrow$ have dipole moment, it must be pyramidal

ZW_3 possess no dipole moment hence it must be planer.

Correct answers are (b) and (d).

18. 5

Sol.



Five atoms lie in the plane.

19. 4

Sol. Lewis bases have a tendency to donate lone pair of electrons. NH_3, H_2O, ROH and $(CH_3)NH_2$ can act as lewis bases.

Correct answer is 4.

20. 4

Sol. Lewis acid have a tendency to accept electron pair and they are electron deficient species H^+, BF_3, AlH_3.

Correct answer is 4.

×××××

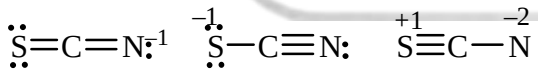
QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 10

1. The ONO angle is maximum is:
   (a) HNO_3 (b) NO_2^+ (c) HNO_2 (d) NO_2
2. Consider the following statement:
   1. Steric number '7' gives sp^3d^3 hybridization.
   2. ClF_3 at least one bond angle is exactly 160°
   3. lone pair does not cause any distortion in bond angle.
   (a) TFF (b) TTF (c) FTF (d) TTT
3. All the following species have all their bonding length identical except:
   (a) AsF_3 (b) AsF_4^- (c) AsF_4^+ (d) $AsF_6^\ominus$
4. Which one of the highest bond angle:
   (a) NH_3 (b) PH_3 (c) H_2O (d) CH_4
5. Which of the following contain both electrovalent and covalent bond?
   (a) CH_4 (b) H_2O_2 (c) NH_4Cl (d) None
6. In the thiocyanate ions $SCN^\ominus$, three resonating structure one possible with electron-dot method shown in figure.



   (X) (Y) (Z)

   The decreasing order of % contribution in resonance hybrid is:
   (a) y > x > z (b) y > z > x (c) z > x > y (d) x = y = z
7. The correct order of C – N bond length in the given compound is:
   (P) P : CH_3CN (Q) HNCO (R) CH_3eONH_2
   (a) P > Q > R (b) P = Q = R (c) R > Q > P (d) R > P > Q
8. The bent of v-shaped molecule can be resulted from which of the following hybridization.
   (a) $-sp^3$ (b) sp^2 (c) Both a and b (d) None of these
9. Which of the following should have pyramidal shape:
   (a) $[ClOF_2)^+$ (b) ICl_3 (c) $[BrCl]^\ominus$ (d) I_3^+

10. The correct order of bond angle is:
(a) $H_2S < NH_3 < BF_3 < CH_4$ (b) $NH_3 < H_2S < CH_4 < BF_3$
(c) $H_2S < NH_3 < CH_4 < BF_3$ (d) $H_2S < CH_4 < NH_3 < BF_3$

11. According the following in the increasing order of deviation from normal tetrahedral:
(a) $P_4 < PH_3 < H_2O$ (b) $PH_3 < H_2O < P_4$
(c) $P_4 < H_2O < PH_3$ (d) $H_2O < PH_3 < P_4$

12. Identify the correct statement:
(a) single N – N bond is stronger than single P – P bond.
(b) single N – N bond is weaker than single P – P bond.
(c) N = N is weaker than P = P
(d) None of these

13. How many S – S bond, S – O – S bond, σ-bond, π-bond are present in trimer of sulphur.
(a) 0, 3, 16, 2 (b) 0, 3, 17, 6 (c) 0, 6, 12, 16 (d) 0, 4, 12, 6

Ans. (b)

14. The shape of XeF_3^p is _____.
(a) Trigonal planar (b) Pyramidal (c) Bent T-shaped (d) See-saw

15. Which of the following molecule(s) is/are having a see-saw geometry?
(a) SF_4 (b) ClF_3 (c) BrF_5 (d) $TeCl_4$

16. Select the correct order of bond angle:
(a) $PI_3 > PBr_3 > PCl_3 > PF_3$ (b) $H_2O > OF_2$
(c) $NH_3 > NF_3$ (d) $OCl_2 < OF_2$

17. Select the correct order of bond angle:
(a) $NH_3 > PH_3 > AsH_3 > SbH_3 > BiH_3$ (b) $H_2O > H_2S > H_2Se > H_2Te$
(c) $BF_3 = BCl_3 = BBr_3 = BI_3$ (d) $BF_3 < BCl_3 < BBr_3 < BI_3$

18. Find the number of reaction(s) in which cordinate bond is/are formed in product side:
(a) $BF_3 + F^{\ominus} \rightarrow BF_4^{-1}$ (b) $NH_3 + H^+ \rightarrow NH_4^+$ (c) $HF + SbF_5 \rightarrow HSbF_0^-$
(d) $H_2O + H^+ \rightarrow H_2O^+$ (e) $PCl_3 + Cl^{\ominus} \rightarrow PCl_4^{\ominus}$

19. Find the number of molecule(s) which do not exist:
NCl_3, PCl_3, PCl_5, NCl_5, OF_2, OF_4, OF_5

20. The dipole moment of HCl is 1.03Δ, if H – Cl bond distance is 1.26 Å. What is the percentage of ionic character in the H – Cl bond _____.

××××

QUANTA CHEMISTRY
An Institute of Chemical Sciences

ANSWER KEY

1.	(b)	8.	(c)	15.	(a, d)
2.	(a)	9.	(a)	16.	(a, b, c, d)
3.	(b)	10.	(c)	17.	(a, b, c)
4.	(d)	11.	(d)	18.	4
5.	(c)	12.	(b)	19.	3
6.	(a)	13.	(b)	20.	17%
7.	(c)	14.	(c)		

HINTS & SOLUTIONS

1. (b)

Sol. ONO bond angle will be maximum where N in the given molecule is sp hybridized.

$NO_2^+ \Rightarrow [O \leftarrow N = O]^+$ is sp – hybridized with bond angle of 180º.

Correct option is (b)

2. (a)

Sol. sp^3d^3 hybridization is for steric number 7.

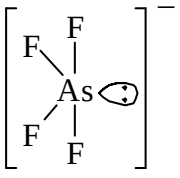
No bond angle in ClF_3 is exactly 160º.

Lone pair causes distortion in bond angle.

Correct option is (a)

3. (b)

Sol. AsF_4^- have TBP geometry in which two F atoms are at equitorial position while other two are at axial position.



Correct option is (b)

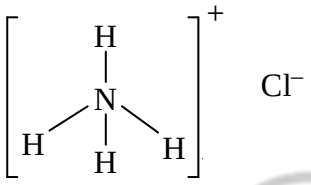
4. (d)

Sol. CH_4 being ideal tetrahedral have highest bond angle among the other tetrahedral species NH_3 and H_2O while PH_3 being a drago molecule have a bond angle of 90º.

Correct option is (d)

5. (c)

Sol. Electrovalent bond means ionic bond. NH_4Cl has electrovalent as well as covalent bond. NH_4Cl exists as NH_4^+ exists as NH_4^+ and Cl^-.



Correct option is (c)

6. (a)

7. (c)

Sol. The order of bond length depends apon % s – character. Higher the %s character, shorter will be the bond.

bond nature (triple bond) (double bond) (single bond)

$\therefore$ Bond length $\propto \frac{1}{\%s - character}$

%s character $\Rightarrow (\equiv) > (=) > (-)$

Correct option is (c)

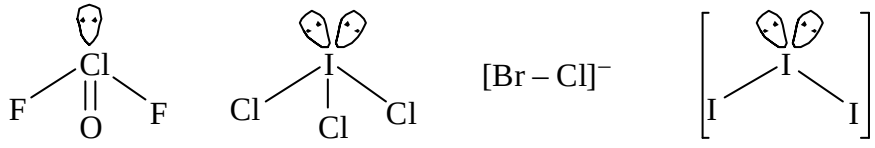
8. (c)

Sol. sp^3 and sp^2 hybridized molecules both can result in bent or v-shaped molecules. Example – H_2O (sp^3 – hybridized) while $SnCl_2$ being sp^2 hybridized is also bent like H_2O.

Correct option is (c)

9. (a)

Sol.



(Pyramidal) (Bent) (Bent)

10. (c)

Sol. Bond angle $\propto$ % s – character

VSEPR rules for bond angle prediction:

(i) Bond angle $\propto \frac{1}{\text{No. of lone pair on central atom}}$

(ii) Bond angle $\propto$ electronegativity of central atom

(iii) Bond angle $\propto \frac{1}{\text{electronegativity of side atom}}$

$\therefore BF_3 > CH_4 > NH_3 > H_2S$

Correct option is (c)

11. (d)

Sol. Ideal tetrahedral bond angle is 109°28´. More deviation from this bond angle, more will be deviation from normal tetrahedral P_4 has bond angle of only 60° while PH_3 and H_2O have 93° and 104.5° respectively.

Correct option is (d)

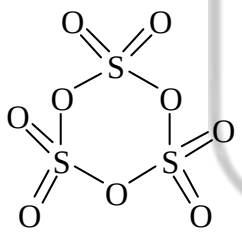
12. (b)

Sol. N – N single bond is weaker than P – P bond due to smaller size of N as compared to P. Smaller size of N leads to smaller N – N bond length. As a result, the lon pair of electrons on both the N atoms repel each other leading to unstability or weakening of N – N bond. Because of larger P atom, this makes P – P bond length more and lone – pair lone pair repulsion less.

Correct option is (b)

13. (b)

Sol.



S – S bond = zero

S – O – S bonds = 3

σ – bond = 12

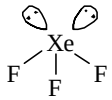
π – bond = 6

Correct option is (b)

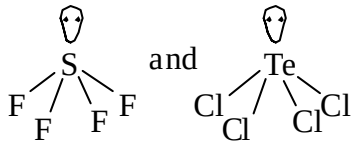
14. (c)

Sol. Shape of XeF_3^+:

in bent T-shape



15. (a, d)

Sol. 

Both have sec – saw geometry.

Correct option is (a) and (d)

16. (a, b, c, d)

Sol. Bond angle prediction according to VSEPR theory:

(i) Bond angle

(ii) Bond angle

17. (a, b, c)

18. 4

19. 3

20. 17%?

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 11

1. Which of the following species used both set of d-orbital in hybridization of central atom.
   (a) PBr_4^+ (b) PCl_4^Θ (c) ICl_4^Θ (d) None
2. Consider the following compounds and select the incorrect statement from the following:
   NH_3, PH_3, H_2S, SO_2, SO_3, BF_3, PCl_3, IF_7, P_4, H_2
   (a) Six molecules out of given compound involves hybridization
   (b) Three molecules are hyper valent compound.
   (c) Six-molecules out of above compound and non-planar in structure.
   (d) Two molecules out of given compound involves ($d\pi - d\pi$) bonding as well as also involve ($p\pi - p\pi$) bonding.
3. FASF bond angle in AsF_3Cl_3 molecule is:
   (a) 90° to 180° (b) 120° (c) 90° (d) 180°
4. In which of the following species the bond are non-directional?
   (a) NCl_3 (b) RbCl (c) $BeCl_3$ (d) BCl_3
5. C_2H_2 is isostructural with
   (a) H_2O_2 (b) NO_2 (c) $SnCl_2$ (d) CO_2
6. Which of the following halides is inert towards hydrolysis at room temperature?
   (a) $SiCl_4$ (b) PCl_3 (c) NCl_3 (d) NF_3
7. The correct order of increasing bond angles is:
   (a) $OF_2 < ClO_2 < H_2O < Cl_2O$ (b) $OF_2 < H_2O < Cl_2O < ClO_2$
   (c) $OF_2 < H_2O < ClO_2 < Cl_2O$ (d) $ClO_2 < OF_2 < H_2O < Cl_2O$
8. In which of the following cases C – C bond length will be highest?
   (a) $CH_3 - CF_3$ (b) $FCH_2 - CH_2F$ (c) $F_2CH - CHF_2$ (d) $CF_3 - CF_3$
9. According to VSEPR model, the shape of $[XeOF_5]$ is:
   (a) octahedral
   (b) square pyramidal
   (c) trigonal bipyramidal
   (d) pentagonal mono pyramidal

10. The correct non linear and iso-structural pair is ____.
(a) Scl_2 and $I_2^{\ominus}$ (b) SCl_2 and I_2^{+} (c) SCl_2 and ClF_2 (d) I_3^{+} and $ClF_2^{\ominus}$

11. The lone pair, and identical in the pairs:
(a) XeF_4, ClF_3 (b) XeO_4, $ISl_4^{\ominus}$ (c) $XeCl_2F_2$, $ICl_a^{\ominus}$ (d) XeO_4, ClF_3

12. CO_3^{2-}, SO_3, XeO_3 and NO_3^{-} have planar structure:
(a) CO_3^{2-}, SO_3, XeO_3 (b) CO_3^{2-}, XeO_3, NO_3^{-}
(c) CO_3^{2-}, XeO_3, NO_3^{-} (d) CO_5^{2-}, SO_3, NO_3^{-}

13. The size of d-orbital in Si, P, S and Cl follow the order
(a) Cl > S > P > Si (b) Cl > P > S > Si (c) P > S > Si > Cl (d) Si > P > S > Cl

14. Among the following pairs, those in which both species have similar structure are:
(i) $N_3^{\ominus}$, XeF_2 (ii) $[ClF_2]^{+}$ $(ICl_2]$ (iii) $(ICl_4]^{-}$ $[PtCl_4]^{2-}$ (iv) XeO_3, SO_3
(a) I and II only (b) I and III only (c) I, II and III only (d) II, III and IV only

15. Which of the following molecule has/have structure similar to NH_3?
(a) PH_3 (b) H_3C^{+} (c) SeF_3^{+} (d) $\overset{\oplus}{C}H_3$

16. Which of the following molecule(s) is/are having two different types of bond length?
(a) PF_5 (b) PCl_5 (c) IF_7 (d) SF_6

17. Which of the following molecule(s) is/are having a square pyramidal geometry?
(a) $TeF_5^{\ominus}$ (b) $XeOF_4$ (c) IF_5 (d) $XeF_5^{\oplus}$

18. The dipole moment of HBr is 2.60×10^{-30} cm and the interatomic spacing is 1.41 Å. What is the per cent ionic character of HBr? _____

19. Find the ratio of the total number of σ bonds to lone pair of sp^2-hybrid orbital in $C_3N_3(N_3)_3$ ____.

20. Find the number of molecule(s) having tetrahedral geometry from the following. _____.
OPF_3, $S_2O_3^{2-}$, XeO_4, SF_4, $TeCl_4$, $NHA^{\oplus}$

××××

QUANTA CHEMISTRY
An Institute of Chemical Sciences

ANSWER KEY

1.	(c)	8.	(b)	15.	(a, b, c, d)
2.	(c)	9.	(d)	16.	(a, b, c, d)
3.	(a)	10.	(b)	17.	(a, b, c, d)
4.	(b)	11.	(a)	18.	11.5%s
5.	(d)	12.	(d)	19.	5
6.	(d)	13.	(d)	20.	4
7.	(b)	14.	(b)		

HINTS & SOLUTIONS

1. (c)

Sol. PCl_4^{Θ} is octahedral geometry (sp^3d^2) and the d-orbitals used are $d_{x^2-y^2}$ and d_{z^2} and shape is square planar. Other two species PBr_4^+ and PCl_4^{Θ} have steric number are 4 and 5 respectively.
Correct option is (c)

2. (c)

3. (a)

4. (b)

5. (d)

Sol. H – C ≡ C – H (linear) is isostructural with CO_2, O = C = O (linear)
Correct option is (d)

6. (d)

7. (b)

Sol. The correct order of bond angle is –

$$\underset{(11.6)}{ClO_2} > \underset{\text{NBEPR dominates}}{Cl_2O} > \underset{\text{Bond angle}}{H_2O} > OF_2 \propto \frac{1}{\text{electronegativity of side atom}}$$

Correct option is (b)

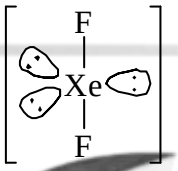
8. (b)
9. (d)
10. (b)
11. (a)
12. (d)
13. (d)

Sol. On moving from left to right in a periodic table, effective nuclear charge hence size of orbitals decreases.

$\therefore$ Size of d-orbitals : Si > P > S > Cl

Correct option is (d)

14. (b)

Sol. $N_3^{\ominus} \Rightarrow \overset{\ominus}{N}=\overset{\oplus}{N}=\overset{\ominus}{N}$, $XeF_2 \Rightarrow$ 

Both are linear.

$ICl_4^{\ominus}$ and $[PtCl_4]^{2-}$ both are square planar

Correct option is (b)

15. (a, b, c, d)
16. (a, b, c, d)
17. (a, b, c, d)
18. 11.5%s
19. 5
20. 4

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 12

1. The species having pyramidal shape is

   (a) SO_3 (b) BrF_3 (c) SiO_3^{2-} (d) OsF_2

2. According to VBT, which of the following overlapping result in π-type covalent bond in O_2 formation of Z-axis is internuclear axis:

   (i) 2s – 2s (ii) $2p_x - 2p_x$ (iii) 1s – 1s (iv) $2p_y - 2p_y$

   (v) $2p_3 - 2p_3$

   (a) i, iii (b) ii, v (c) ii, iv (d) iv, v

3. Which set contain no ionic species?

   (a) NH_4Cl, OF_2, H_2S (b) CO_2, CCl_4, Cl_2

   (c) BF_3, AlF_3, TiF_3 (d) Z_2, CuO, CH_3Cl

4. The correct decreasing order of nearest bond angle:

   (a) $ClF_3 > PF_3 > NF_3 > BF_3$ (b) $BF_3 > PF_3 > NF_3 > ClP_3$

   (c) $BF_3 > ClF_3 > PF_3 > NF_3$ (d) $BF_3 > NF_3 > PF_3 > ClF_3$

5. Molecule type number of L-P on central atom A.

   I. AB_2 (p) zero

   II. AB_3 (q) one

   III. AB_4 (r) two

   (s) three

   Set the condition when AB_2, AB_3, AB_4 type neutral molecule having Non-zero dipole moment.

   (a) I = q, r (b) II – q, r (c) III = q (d) All of these

6. The incorrect order of bond angle:

   (a) $CO_2 > CO_3^{2-} > CF_2Cl_2$ (b) $NO_2^+ > NO_3^- > NO_2^-$

   (c) $XeF_2 > XeF_4 > XeO_4$ (d) $PH_3 > ASH_3 > SbH_3$

7. In SNF_3, the ∠FSF should be:

   (a) less than 120° and more than 180° 28.

   (b) less than 109° 28

(c) less than 180º and more then 120º

(d) Exactly equal to 109º 28.

8. Which of the following compound ion is planar.

(a) SFS^- (b) SF_4 (c) OSF_4 (d) SF_2

9. Geometry of $TeCl_4$ is:

(a) see - saw (b) folded square (c) distorted Td (d) All of these

10. In which of the following d-orbital are not used by central atoms in hybridisation:

(a) $PF_5(s)$ (b) $PCl_5(g)$ (c) $PBr_5(s)$ (d) $XeF_6(s)$

11. Total number of vacant orbital in valency shell Br when it forms maximum covalent bonds:

(a) 9 (b) 2 (c) 3 (d) 5

12. Molecule which does not contain any F – X – F bond angle which is less 90º (X = central atom)

(a) IF_7 (b) BrF_3 (c) PF_5 (d) SF_4

13. Which of the following does not have $P\pi - P\pi$ bond_____.

(a) SO_3 (b) NO_3^- (c) $B_3N_3H_6$ (d) $SOCl_2$

14. Which of the following change CH_4 can not cause the change in bond angle?

(a) On replacing C by Si

(b) On replacing one of the 'H' by F atom

(c) On removing H^+ from molecule

(d) On replacing all the – H by I.

15. In which of the following hybridisation lone pair are not observed on opposite position?

(a) sp^3 (b) sp^3d (c) sp^3d^2 (d) sp^3d^3

16. Select the correct statement for $AbnL_2$:

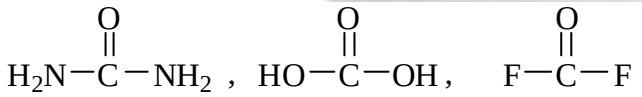
A $\rightarrow$ central atom, L $\rightarrow$ Lone pair of $e^{\ominus}$ and n $\rightarrow$ monovalent atom.

(a) Molecule will be planar and non polar when $\eta = 4$

(b) Molecule will be non planar and polar when $\eta = 3$

(c) Molecule will be planar and polar when $\eta = 2$

(d) Bond polarity is equal to molecularity polarity when $\eta = 2$

17.  have:

(a) different number of lone pair (b) different no. of total bond pair

(c) same no. of electrons (d) same no. of σ bond pair

18. Sum of $p\pi - p\pi$ bond in $SO_2(g)$ and $SO_3(g)$ is _____.

19. Total no. of bonds in TF_7 which are at 72º 10_____.

20. No. of lone pair(s) in $COCl_2$ molecule is_____.

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	d
2.	c
3.	b
4.	d
5.	d
6.	c
7.	b
8.	d
9.	d
10.	(c)
11.	a
12.	c
13.	d
14.	a, d
15.	a, b
17.	c
18.	3
19.	5
20.	8

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 13

1. Which of the following would result in the formation of strongest π-bond if the molecular axis is X-axis?
   (a) $2p_x + 2p_x$ (b) $2p_y + 2p_y$ (c) $2p_x + 3d_{xy}$ (d) $2p_z + 4p_z$
2. In which of the following species pπ – dπ bond is present but pπ – pπ bond is absent?
   (a) SiH_4 (b) CS_2 (c) SO_2 (d) SO_2Cl_2
3. In which of the following pairs, the hybridisation of central atom is same, but geometry is not the same.
   (a) SO_3, CO_3^{2-} (b) $SO_3^{2-} + NH_3$ (c) PCl_5, $PoCl_3$ (d) XeF_2, ICl_3
4. In which of the following, all central atom-surrounding atom bound is not a equal length?
   (a) XeF_2 (b) XeF_4 (c) $PF_{5\backslash}$ (d) BF_3
5. Given a molecule with general formula AB_1, which one of the following would be most useful in determining whether the molecule was bent or linear?
   (a) Electronegativity of atom (b) Bond energies of bond
   (c) Ionization energies of atom (d) Dipole moment of molecule
6. For given element which pair have highest electronegativity difference?
   (a) C and I (b) P and H (c) N and Cl (d) O and F
7. If YZ plane contain all the atom of formaldehyde (H_2CO). Find the nodal plane of π-bond in formaldehyde ___
   (a) XY (b) YZ (c) XZ (d) Not-predictable
8. Which of the following molecular geometry is not produced by sp^3d hybridisation?
   (a) Tringular planar (b) See-saw (c) 'T' Shape (d) Linear
9. Which of the following option the change in the bond angle in given reaction?
   $BF_3 \rightarrow BF_4^-$
   (a) 120° (b) 109°28′ (c) 107°2′ (d) 60
10. AX_3 type of molecules are non-planar when there is/are lone pair on (A).
    (a) One (b) Two (c) Zero (d) None of these

11. Total number of edge present in CF_4 polyhedron is ____.
(a) Six (b) Four (c) Three (d) Five

12. In AB_xL_y (sp^3d-hybridisation of A) have 'T' shape geometry. What will be the geometry of molecule if 'A' from AB_yL_x types of molecules (B $\rightarrow$ bond, L $\rightarrow$ lone pair).
(a) 'T' shape (b) See-saw (c) T.B.P (d) Linear

13. Select the correct statement about CH_4:
(a) All the hybrid orbitals of carbon are equivalent
(b) All the hybrid orbitals of carbon have 25% is property
(c) All the hybrid orbital of carbon are projected at four vertex of a regular tetrahedron.
(d) All are correct statement.

14. In which species the hybrid state of central atom is/are sp^3d?
(a) I_3^+ (b) SF_4 (c) PF_5 (d) IF_5

15. A molecule XY_z contain 2σ, 2π bond and lone pair of electron in the valance shell of X. The arrangement of lone pair and bond pair is:
(a) square pyramidal (b) linear (c) trigonal planar (d) unpredictable

16. Which of the following pairs of species have identical shapes?
(a) NO_2^+, NO_2^- (b) PCl_5, BrF_5 (c) XeF_4 and ICl_4^- (d) $TeCl_4$, XeO_4

17. Which of the following molecules or ions is/are linear?
(a) $BeCl_2$ (b) ICl_2^- (c) CS_2 (d) ICl_2^+

18. Total no. of plane in CH_4 which contain 3 atom in a plane with carbon is _____.

19. Ratio of σ-bond and π-bond in benzene molecule _____.

20. Select the number of orbital which can produced 'π' bond when overlap with an S-orbitals ____
P_x, P_y, P_z, d_{xy}, d_{yz}.

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	(b)
2.	(b)
3.	(d)
4.	(c)
5.	(D)
6.	(d)
7.	(b)
8.	(a)
9.	(c)
10.	(a)
11.	(a)
12.	(d)
13.	(d)
14.	(b, c)
15.	(c)
16.	(c)
17.	(a, b, c)
18.	6
19.	4
20.	0

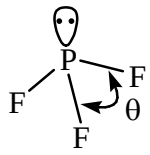
QUANTA CHEMISTRY

An Institute of Chemical Sciences

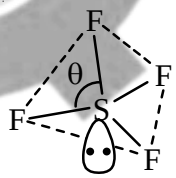
CHEMICAL BONDING

DPP- 14

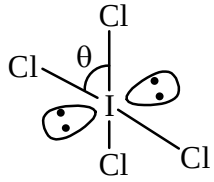
1. I_3^+ and $I_3^{\ominus}$ have same:
   (a) Geometry (b) No. of lone pair (s)
   (c) Bond angle (d) None of these
2. Molecular plane of C_2H_4 does not contain:
   (a) C – C – Bond (b) C – H σ Bond
   (c) all plane have of C_2H_4 atom (d) π-electron in plane
3. In which of the following molecule/ion their is a coordinate type π-bond is present?
   (a) CO (b) NH^+_4 (c) BF^-_4 (d) All of these
4. Which of the following structure is correctly drawn according to fundamental idea of VSEPR theory?

   (a) 

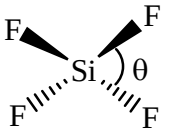
   θ = Greater than

   (b) 

   θ less than 90°

   (c) 

   θ = 90°

   (d) 

   θ = 90°

5. In which of the following pair of molecules/ions, both the species are not likely to exist.
   (a) H_2^{2+}, He_2 (b) H_2^-, He_2^{2+} (c) H_2^+, He_2^{2-} (d) H_2^-, He_2^{2-}
6. Stability of species Li_2, Li_2^-, Li_2^+ increase in the order:
   (a) $Li_2 < Li_2^- < Li_2^+$ (b) $Li_2^- < Li_2 < Li_2^{2+}$ (c) $Li_2 < Li_2^+ < Li_2^-$ (d) $Li_2^2 < Li_2^+ < Li_2$
7. Which orbitals of two atom produced (δ) bond?

(a) $d_{z^2} \rightarrow$ Overlap on Z-axis $\leftarrow d_{z^2}$ (b) $d_{zy} \rightarrow$ Overlap on X-axis $\leftarrow d_{xy}$

(c) $d_{x^2-y^2} \rightarrow$ Overlap on Y-axis $\leftarrow d_{x^2-y^2}$ (d) $d_{xz} \rightarrow$ Overlap on Y-axis $\leftarrow d_{xz}$

8. Which of the following molecular shape can be obtained from octahedral electron geometry of a central atom.
(a) Square planar (b) Octahedral
(c) Trigonal pyramidal (d) Square pyramidal

9. Number of hybrid orbital of Xe which contain lone pair is/are maximum in which of the following molecule.
(a) XeF_4 (b) XeO_3 (c) XeF_6 (d) XeF_2

10. All alumini (f) atoms are in same plane in:
(a) CHF_3 (b) ClF_3 (c) $XeOF_4$ (d) All of these

11. Nodal plane of all the π-bonds in the same plane:
(a) C_6H_6 (b) CO_2 (c) $H_2C = C = CH_2$ (d) N_2

12. Select hybridisation which have non-planar geometry when all one bond pair, but planar when there are 2 lone pairs on central atom:
(a) sp^3 (b) sp^3d (c) sp^3d^2 (d) all of these

13. Assume that BrF_3, in liquid phase intermolecularly exchange one $F^{\ominus}$ ion to give an ion pair, then which of the following statement(s) is/are correct?
(a) cation is sp^3 hybrid and anion is sp^3d^2 hybrid.
(b) cation and anion both are plannar.
(c) cation is non-planar and anion is planar.
(d) cation is planar and anion is non-planar.

14. An atom which have $3d^2$, $3p^1$, $3d^0$ ground state electronic configuration of outermost shell. Select the correct statement..
(a) it form MX_3 type covalent halides
(b) it can form MX_4^- type of ion (X-halogen)
(c) it can form MX_6^{3-} type of ion (X-halogen)
(d) it can form M_2X_6 type molecular (X-halogen)

15. According to VB^{-1} in XeF_2, Xe used fire sp^3d hybridise orbital for molecule formation. Select correct statement for XeF_2.
(a) Three sp^3d orbitals used for covalent bonding with F.
(b) Three sp^3d orbital occupied L.P of Xe.
(c) Two sp^3d orbitals used for covalent bonding with F.
(d) Two sp^3d orbital used by lone pair of Xe.

16. Select species which is/are isostructural with NNO (laughing gas)
(a) $ONO^{\ominus}$ (b) $NCO^{\ominus}$ (c) $NNN^{\ominus}$ (d) NCN^{2-}

17. All the valency shell orbitals of central atom used for bond in.
(a) BF_3 (b) $BeCl_2$ (c) CH_4 (d) CO_2

18. The total number of edge in T.B.P polyhedron is ____.
19. The number of faces in $SF_5^{\oplus}$ ions polyhedron is ___.
20. Total number of vacant orbital in valency shell of sulphur when it undergoes formation of SF_4 is _____.

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	(d)
2.	(d)
3.	(a)
4.	(c)
5.	(a)
6.	(d)
7.	(d)
8.	(c)
9.	(d)
10.	(d)
11.	(a)
12.	(a)
13.	(a, b)
14.	(a, b, c, d)
15.	(b, c)
16.	(b, c, d)
17.	(c, d)
18.	9
19.	6
20.	4

QUANTA CHEMISTRY

An Institute of Chemical Sciences

CHEMICAL BONDING

DPP- 15

1. State of hybridisation of sulphur, carbon-1, and C – 2 in $F_3S\underset{(1)}{C}\underset{(2)}{C}F_3$ respectively.

   (a) sp^3, sp^3, sp^3 (b) sp^3, sp^2, sp^3 (c) sp^3d, sp, sp^3 (d) sp^3, sp, sp^3

2. Select the correct statement for BrF_5:

   (a) All flourine atoms are in same plane. (b) Four 'F' atoms and 'Br' is in the same plane.

   (c) Four 'F' atoms are in same plane. (d) It has at F – Br – F bond angle at 90°

3. Total number of planes which contain 4 atoms in a plane the maximum in:

   (a) CH_4 (b) PCl_5 (c) XeF_4 (d) SF_4

4. Two isoelectronic pair are formed on matching.

   (A) Co, $(CN)_2$ (P) SO_2, cyclic $(SO_3)_3$

   (B) $(NH_2)_2$ Co, Co_2 (Q) ICl_2^+, MnO_4^-

   (C) $TeCl_2$, CrO_4^{2-} (R) $(CH_3)_2$ CO, NO_2

   (D) ClO_3^+, Si_3Og^{2-} (S) BF, B_2O_3

   According to above statement which of the following option is correct.

   (a) A – D, B – Q, C – R, D – S (b) A – S, B – Q, C – R, D – P

   (c) A – S, B – R, C – Q, D – P (d) A – P, B – R, C – Q, D – S

5. In ICl_2^+, ICl_2^-, ICl_4^- sum of bond pair and lone pair on each iodine atom are respectively.

   (a) 2 and 2 (b) 2, 3 and 2 (c) 4, 5 and 4 (d) 4, 5 and 6

6. Consider a P_y-orbital of an atom and identify correct statement:

   (a) S-orbital of another atom produce π-bond Y is bond formation axis.

   (b) P_y orbital of another atom produce σ-bond when X is the bond formation axis.

   (c) P_2 orbital of another atom produced π-bond when X is bond formation axis.

   (d) d_{xy} orbital of another atom produce π-bond when 'X' is the bond formation axis.

7. Which of the following order is correct for dipole moment?

   (a) $CH_3F > CH_3Cl > CH_3Br > CH_3I$ (b) $CH_3Cl > CH_3Br > CH_3F > CH_3I$

   (c) $CH_3Br > CH_3Cl > CH_3I > CH_3F$ (d) $CH_3Cl > CH_3F > CH_3Br > CH_3I$

8. Out of given molecules, how many molecules, contain two-pi bonds in between carbon atoms.
CaC_2, C_2Cl_2, C_2HCl, $C_2H_2Cl_2$, C_2HCl_5?
(a) Two (b) Three (c) Four (d) Only one

9. In $CuSO_4.5H_2O$ total number of H_2O molecule which form coordinate bond with metal is:
(a) 2 (b) 4 (c) 5 (d) 0

10. The d-orbital which are one involved in hybridisation of central atom in ICl_4^-:
(a) $d_{z^2}, d_{x^2-y^2}$ (b) $d_{x^2-y^2}, d_{xy}, d_{yz}, d_{zx}$ (c) $d_{z^2}, d_{xy}, d_{yz}, d_{xz}$ (d) d_{xy}, d_{xz}, d_{yz}

11. Which of the following structure of $(CN_2)^{2-}$ is incorrect?
(a) $:\ddot{\underset{\cdot\cdot}{N}}^{2}-C\equiv N:$ (b) $:\underset{\cdot\cdot}{N}=C=\underset{\cdot\cdot}{N}:$ (c) $:N\equiv C-\ddot{\underset{\cdot\cdot}{N}}:^{2-}$ (d) $\ddot{\underset{\cdot\cdot}{N}}=C=\ddot{\underset{\cdot\cdot}{N}}:^{-}$

12. Consider the following statements:
(i) Coralancy of hydrogen can't be more than one.
(ii) Nitrogen can't form more than four covalent bonds.
(iii) In all the possible non-cyclic lewis structure of azide ion (N_3^-) central nitrogen has covalancy of four.
(iv) Maximum covalency of sulphur is two as it has two unpaired electron in its valence shell.
Using T for true and F for false. Correct answer is
(a) FTTF (b) TTTT (c) TFTF (d) TTTF

13. What is the formal change on carbon in CO and CO_2 respectively?
(a) –1, zero (b) –1, + 2 (c) –2, +4 (d) –1, +4

14. $KK\sigma 2s^2\sigma^* 2s^2 \begin{cases} \pi^2 P_{y^2} \ \ \sigma^2 P_{x^2} \\ \pi^2 P_{z^2} \end{cases}$ above electronic
distribution is observed in:
(a) Atomic nitrogen (b) Molecular nitrogen (c) O_2^{2+} ion (d) C_2^{2-} ions

15. Molecule ion in which both the lone pairs are opposite to each other.
(a) XeF_4 (b) SF_2 (c) ClF_3 (d) $XeF_5^{\ominus}$

16. Select correct order of bond energy:
(a) $F_2 > Cl_2 > Br_2 > I_2$ (X – X) (b) $N_2 > N_2H_2 > N_2H_4$ (N – N)
(c) $O_2 > O_3 > H_2O_2$ (O – O) (d) $C_2H_4 > C_2H_4 > C_2H_6$ (C – C)

17. Hybrid orbital of an atom have $(sp^3)^2$, $(sp^3)^1$, $(sp^3)^1$, $(sp^3)^1$. Electronic distribution. Select the correct statement for molecule which is formed by overlapping of required F-atoms.
(a) Molecule will be non-planar (b) Molecule will be planar
(c) Molecule have total 10 lone pairs (d) Bond angle will be less than 10%.

18. $\underset{X}{PF_3} \xrightarrow[\Delta]{F_2(Excess)} \underset{Y}{PF_5} \xrightarrow{F^{\ominus}} \underset{(Z)}{PF_6^{\ominus}}$

Find the sum of vacant orbital in the valance shell of phosphrous in (X) and (Z) species of above reaction ____.

19. Number of lone pair-bond pair repulsion of 90° are (P) in $I_3^{\ominus}$ are (Q) in ICl_4^-. Find difference of (P – Q) ____.

20. Select number of species which have pyramidal type of structure with square base.

NF_3, SoF_2, IF_5, IoF_4, IO_3^-, XeF_5^-, XeF_5^+, XeO_3

××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWER KEY

1.	(d)
2.	(c)
3.	(b)
4.	(c)
5.	(b)
6.	(d)
7.	(d)
8.	()
9.	(b)
10.	(d)
11.	(d)
12.	(d)
13.	(a)
14.	(b, d)
15.	(a, d)
16.	(b, c, d)
17.	(a, b, c, d)
18.	7
19.	2
20.	3

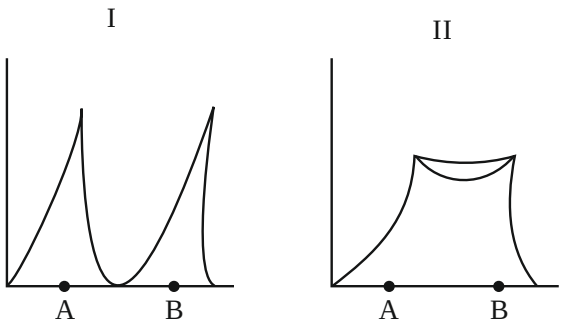
QUANTA CHEMISTRY

An Institute of Chemical Sciences

Assignment Sheet - MOLECULAR ORBITAL THEORY

1. If the sign of wave function is unchanged when the orbital is reflected about its centre, the orbital is
   (a) Gerade (b) Ungerade
   (c) Gerade as well as ungerade (d) None of mentioned
2. The filling of molecular orbital takes place according to
   (a) The Aufbau principle (b) Pauli exclusion principle
   (c) Hund's rule of maximum multiplicity (d) All of the mentioned.
3. Stability increases, as the energy.....
   (a) increases (b) does not change
   (c) decreases (d) increases and then decreases
4. Which of the following is a condition for the combination of atomic orbitals?
   (a) Combining atomic orbitals need not have equal energy.
   (b) Combining atomic orbitals must have symmetry as per molecular axis.
   (c) Combining atomic orbitals must overlap to a minimum extent.
   (d) For combining atomic orbitals, X-axis should be taken as a molecular axis.
5. Take N_A as the number of anti-bonding molecular orbitals and N_B as the number of bonding molecular orbitals. The molecule is stable when:
   (a) N_A is greater than N_B
   (b) N_A is equal to N_B
   (c) N_A is less than N_B
   (d) N_A is greater than or equal to N_B
6. Antibonding molecular orbitals are produced by
   (a) constructive interaction of atomic orbitals.
   (b) destructive interaction of atomic orbitals.
   (c) the overlap of the atomic orbitals of two negative ions.
   (d) All of these

7. Probability (electron charge density) of bonding and anti-bonding molecular orbitals are given.



Select the correct probability.

(a) I bonding, II anti-bonding (b) II bonding, I antibonding

(c) Both I and II bonding (d) Both I and II anti-bonding

8. According to molecular orbital theory, the shape and size of a molecular orbital depends on____

(a) Shape and size of the combining atomic orbitals

(b) Numbers of the combining atomic orbitals

(c) Orientation of the combining atomic orbitals

(d) All of the mentioned.

9. Which of the following statements are true.

(a) When one considers the molecular orbitals resulting from the overlap of any two specific atomic orbitals, the bonding orbitals are always lower in energy than the antibonding orbitals.

(b) Molecular orbitals are generally described as being more delocalized than hybridized atomic orbitals.

(c) One of the shortcoming of molecular orbital theory is its inability to account for the triple bond in the nitrogen molecule, N_2.

(d) One of the shortcomings of valence bond theory is its inability to account for the paramagnetism of the oxygen molecule, O_2.

10. Which of the following statements is true.

(a) Sigma molecular orbitals are symmetrical around the bonding axis.

(b) Bond order is inversely proportional to bond length.

(c) Antibonding molecular orbital are always ungerade.

(d) Bonding molecular orbitals are always gerade.

11. Which of the following nodal equation is correctly satisfied

(a) $\sigma = \pi$ (b) $\sigma^* = \pi$ (c) $\sigma^* + \pi = \pi^*$ (d) $\sigma^* = \pi^*$

12. Which of the following molecular orbital will be formed P_x and P_y orbital combine along x-axis.

(a) Bonding (b) Non-bonding (c) Antibonding (d) All of these

13. Which of the following statement is correct.

(a) P_z and P_x orbital combines along x-axis axis to from non-bonding molecular orbital.

(b) P_z and P_x orbital combine along x-axis to form bonding molecular orbital.

(c) P_z and P_x orbital combine along z-axis to form bonding orbital.

(d) P_z and P_x orbital combine along y-axis to form bonding orbital.

14. Which of the following statement is true.
(a) S and $d_{x^2 - y^2}$ orbitals combine along x-axis to form σ bond.
(b) S and d_{xy} orbitals combine along y-axis to form σ bond.
(c) S and d_{xy} orbitals combine along z-axis to form σ bond.
(d) S and $d_{x^2 - y^2}$ orbitals combine along y-axis to form σ bond.

15. The bond order of H_2, H_2^+ and H_2^- are respectively
(a) 1, 0.5, 1 (b) 1, 1, 1 (c) 1, 0.5, 0.5 (d) 0.5, 0.5, 0.5

16. The magnetic nature of H_2, H_2^+ and H_2^- is respectively.
(a) Paramagnetic, diamagnetic, diamagnetic
(b) Diamagnetic, paramagnetic, paramagnetic
(c) Diamagnetic, paramagnetic, diamagnetic
(d) Paramagnetic, paramagnetic, paramagnetic

17. Which of the following statement is correct.
(a) F_2 is coloured due to $\sigma \rightarrow \sigma^*$ transition. (b) Cl_2 is colourless
(c) F_2 is colourless (d) Cl_2, Br_2 and I_2 are coloured.

18. Bond order of O_2, F_2, N_2 respectively are .....
(a) 1, 2, 3 (b) 2, 3, 1 (c) 2, 1, 3 (d) 3, 2, 1

19. Arrange the following molecules in decreasing bond length.
(a) $O_2 > O_2^- > O_2^+ > O_2^{2-}$ (b) $O_2^{2-} > O_2^- > O_2 > O_2^+$
(c) $O_2^2 > O_2^- > O_2^+ > O_2$ (d) $O_2^- > O_2^+ > O_2^{2-} > O_2$

20. Arrange the following molecules in the order of increasing stability.
(a) $N_2^+ < N_2 < N_2^- < N_2^{2-}$ (b) $N_2^{2-} < N_2^- < N_2 < N_2^+$
(c) $N_2^{2\neg} < N_2^- < N_2^+ < N_2$ (d) $N_2 < N_2^+ < N_2^- < N_2^{2-}$

21. On the basis of molecules orbital theory, select the most appropriate option.
(a) The bond order of O_2 is 2.5 it is paramagnetic.
(b) The bond order of O_2 is 2 and it is diamagnetic.
(c) The bond order of O_2 is 1.5 and it is paramagnetic.
(d) The bond order of O_2 is 2 and it is paramagnetic.

22. Which of the following molecule does not exist due to its zero bond order?
(a) H_2^+ (b) He_2^+ (c) He_2 (d) H_2^-

23. The relative energies of molecular. orbitals in increasing order have been found to be as follows:
$(\sigma_{1S}) < (\sigma^*_{1S}) < (\sigma_{2S}) < (\sigma^*_{2S}) < (\pi_{2Px} = \pi_{2Py}) < (\sigma_{2Pz}) < (\pi^*_{2Py}) = (\pi^*_{2Pz}) < (\sigma^*_{2Pz})$
(a) For O_2 to Ne_2 (b) For H_2 to N_2 (c) For H_2 to Ne_2 (d) For N_2 to Ne_2

24. Bond order of NO^+ molecule is—
(a) 2 (b) 3 (c) 2.5 (d) 4

25. When O_2 changes to O_2^-, the electron goes to which of the orbitals.
(a) π orbital (b) σ orbital (c) π∗ orbital (d) π∗ orbital

26. O – O bond length is minimum in
(a) O_2^- (b) O_2 (c) O_2^+ (d) O_2^{2-}

27. O_2 molecule is para magnetic because:
(a) Bonding electrons are more than antibonding electrons.
(b) contain unpaired electrons
(c) Bonding electrons are less than antiboding electrons.
(d) Bonding electrons are equal to antibonding electrons.

28. The paramagnetic nature of O_2 molecule is best explained on the basis of .....
(a) Hybridization (b) Valance bond theory
(c) Resonance (d) Molecular Orbital theory

29. Which of the following molecule has the higher bond order?
(a) N_2 (b) O_2 (c) O_2^+ (d) H_2

30. N_2 accepts electron and converts into N_2^-, where does this last electron go?
(a) Bonding π molecular orbital (b) Antibonding π molecular orbital
(c) Sigma antibonding molecular orbital (d) Sigma bonding molecular orbital

31. In O_2, O_2^-, O_2^{2-} molecular species, total number of π-antibonding electron are respectively.
(a) 2, 3, 4 (b) 4, 3, 2 (c) 3, 2, 4 (d) 2, 4, 3

32. The N – N bond distance in $[N_2]^+$ is longer than N_2 this is due to:
(a) loss of electron from $\sigma_g 2_p$ (MO) (b) the loss of electron from π_{2p} (MO)
(c) the gain of electron in σ*2p (MO) (d) None of above

33. Which of the following pair of molecules/ions, both the species are not likely to exist:
(a) H_2^{2+}, He_2 (b) H_2^-, He_2^{2+} (c) H_2^+ (d) H_2^-, He_2^{2-}

34. The HoMo in HF molecule have _____ characteristics:
(a) σ (b) π* (c) non-bonding (d) σ*

35. The total non-bonding electrons in HF molecule are–
(a) 4 (b) 8 (c) 2 (d) zero

36. The LUMO for OH^- ion is–
(a) σ (b) σ* (c) non-bonding (d) π

37. The correct statement about OH^- ions is–
(a) it can behave as only σ-donor (b) it can behave as both σ and π-donor
(c) it can behave as π-acceptor (d) None of these

38. The correct statement among the following is–
(a) OH^- and HF both can behave as π-donors.
(b) OH^- can behave as π-donor.
(c) HF can behave as π-donor.
(d) OH^- and HF can behave as σ-donors only

39. For NO^+ molecule, the nature of lowest unoccupied molecular orbital is—
(a) non-bonding (b) σ* (c) π* (d) π

40. The correct order of N – O bond length is–
(a) $NO > NO^+ > NO^-$ (b) $NO > NO^- > NO^+$
(c) $NO^+ < NO < NO^-$ (d) $NO \approx NO^+ \approx NO^-$

41. The bond order of CN^- is:
(a) 2.5 (b) 3.0 (c) 2.0 (d) 2.75

42. The bond order of OF molecule is—
(a) 1.5 (b) 2.0 (c) 3.5 (d) 3.0

43. On going from $NO \rightarrow NO^+$, the electron is removed from–
(a) σ (b) non-bonding (c) π^* (d) σ^*

44. The bond order in BF molecule is—
(a) 2.0 (b) 2.5 (c) 1 (d) 3.0

45. Consider CN^- molecule and predict the correct statements–
(a) Bond order is 3.5
(b) There are 3 electron pairs in bonding molecular orbitals
(c) CN^- have 13 electrons
(d) The MO diagram would be similar like N_2 molecule

46. HF behave as σ-donor only but not as π-donor because–
(a) the hold of nucleus on e^- is more in case of HF
(b) the hold of nucleus on e^- is less in case of HF
(c) the hold of nucleus on e^- has no role in this
(d) None of these

47. Which of the following statement is correct–
(a) CO is σ-donor only (b) CO is σ-donor & π-donor
(c) CO is σ-donor and π-acceptor (d) CO is π-acceptor only

48. The number of unpaired electrons in BN are–
(a) two (b) three (c) Zero (d) One

49. The number of electrons in HOMO of H_2O are–
(a) One (b) Two (c) Four (d) Three

50. Which of the following statement is correct–
(a) H_2O of OH^- have $2e^-$ each in HOMO.
(b) H_2O has $2e^-$ in HOMO while OH^- have $4e^-$.
(c) H_2O & OH^- have $4e^-$ each in HOMO
(d) None of these

51. Which among the following species involve s-p mixing–
(a) N_2 (b) F_2 (c) Cl_2 (d) Both (a) & (c)

52. The correct statement about CO is—
(a) The LUMO for CO is singly degenerate and it is gerade.
(b) The LUMO for CO is doubly degenerate and it is ungerade.

(c) The LUMO for CO is singly degenerate and it is ungerade.

(d) The LUMO for CO is doubly degenerate and it is gerade.

53. The correct order of bond order is–

(a) $O_2^+ > CN > N_2^-$ (b) $N_2^+ > CN^- > O_2^+$ (c) $O_2^+ = CN = N_2^-$ (d) $O_2^+ < CN < N_2^-$

54. Predict the correct statement about NH_3 –

(a) The HOMO is doubly degenerate is NH_3. (b) The LUMO is singly degenerate in NH_3.

(c) The HOMO is triply degenerate in NH_3. (d) The LUMO is doubly degenerate in NH_3.

55. The correct molecular orbital configuration for SF_6 is–

(a) $1a_1^2, 1t_1^4, 1e^4$ (b) $1a_1^2, 1t_1^6, 1e^4$ (c) $1a_1^2, 1e^4, t_1^6$ (d) $1a_1^2, 1t_1^4, 1e^2$

56. The number of unpaired e^- O_2^-, O_2^+ and BN respectively are–

(a) 2, 2, 1 (b) 1, 2, 1 (c) 1, 1, 0 (d) 0, 1, 0

57. The species having doubly degenerate LUMO are–

(a) BN, CN, O_2 (b) BN, CN, NO^+ (c) CN, NO^+ (d) BN, O_2

58. The correct statement among the following is:

(a) BN and NO are isolectronic (b) CO and NO^+ are isoelectronic

(c) NO and CO are isoelectronic (d) N_2 and O_2^+ are isoelectronic

59. The bond order of NO^+ and no. of electrons matches with which of the following—

(a) N_2 (b) O_2^{2+} (c) C_2^{2+} (d) O_2^+

60. In BH_3, the LUMO is of _____ nature.

(a) σ (b) non-bonding (c) σ* (d) π

61. The HOMO of CO_2 is—

(a) doubly degenerate and gerade (b) singly degenerate and ungerade

(c) non-bonding (d) doubly degenerate and ungerade

62. The HOMO of HF and LUMO of BF molecule respectively are–

(a) non-bonding & non-bonding (b) non-bonding and σ

(c) σ and non-bonding (d) σ* and σ*

×××××

QUANTA CHEMISTRY
An Institute of Chemical Sciences

ANSWERS

1. (a)
2. (d)
3. (c)
4. (b)
5. (c)
6. (b)
7. ()
8. (d)
9. (c)
10. (b)
11. (c)
12. (b)
13. (a)
14. (a)
15. (c)
16. (b)
17. (d)
18. (c)
19. (b)
20. (c)
21. (d)
22. (c)
23. (b)
24. (b)
25. (c)
26. (c)
27. (b)
28. (d)
29. (a)
30. (b)
31. (a)
32. (a)
33. (a)
34. (c)
35. (b)
36. (b)
37. (b)
38. (b)
39. (c)
40. (c)
41. (b)
42. (a)
43. (c)
44. (c)
45. (d)
46. (a)
47. (c)
48. (c)
49. (b)
50. (b)
51. (d)
52. (d)
53. (c)
54. (b)
55. (b)
56. (c)
57. (c)
58. (b)
59. (a)
60. (b)
61. (c)
62. (a)

QUANTA CHEMISTRY
An Institute of Chemical Sciences

Hints & Solutions

1. (a)

Sol. If the sign of the wave function is unchanged when the orbital is reflected about its centre (i.e. x, y and z are replaced by –x, –y and –z), the orbital is gerade.

2. (d)

Sol. According to these principles, molecular orbitals are filled in order of increasing energy. Two electrons in same orbitals cannot have the same set of all four quantum number identical.

3. (c)

Sol. As the stability increases, the energy of orbital decreases. Stability is inversely proportional to the energy.

4. (b)

Sol. Combining atomic orbitals must have symmetry as per molecular axis is true. The combining atomic orbitals must have equal energy, must overlap to the maximum extent and z-axis should be taken as the molecular axis.

5. (c)

Sol. When a molecule consist both bonding molecular orbitals and anti-bonding molecular orbitals, higher the number of bonding orbitals, more is bonding influence and the more stable molecule will be and vice-versa.

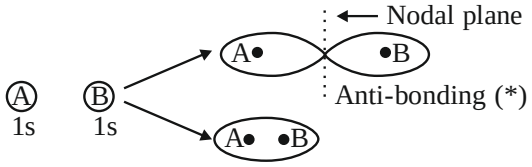
6. (b)

Sol. Destructive interaction of atomic orbitals leads to formation of antibonding molecular orbital.

7. ()

Sol. Electron-charge density in a bonding molecular orbital in high in the internuclear region as shown in II.

In an anti-bonding molecular orbital, it is high in parts of molecule away from the inter nuclear region.



8. (d)

Sol. The shape and size of a molecular orbital depend upon the shape, size, number and orientation of the combining atomic orbitals.

9. (c)

Sol. Molecular orbital theory successfully explain the triple bond in the nitrogen molecule, N_2.

10. (b)

Sol. Sigma molecular orbitals are symmetrical around the bonding axis in pi-molecular orbitals are not symmetrical around the bonding axis.

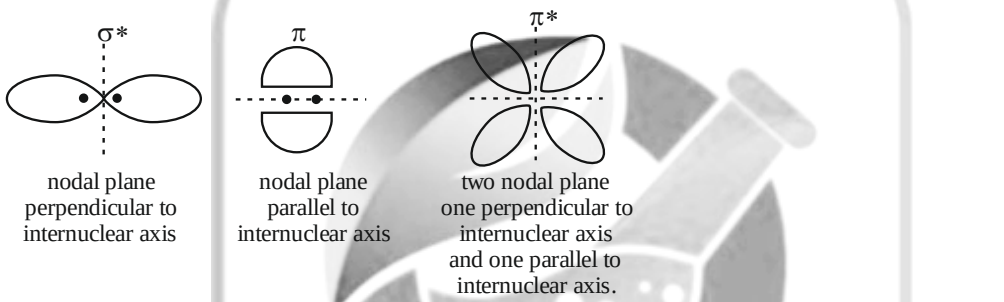
Bond order is inversely proportional to bond length.

Bond length increases then bond order decreases.

It is not necessary that all bonding orbitals are gerade as pi-bonding molecular orbital is ungerade but σ-bonding molecular orbital in gerade.

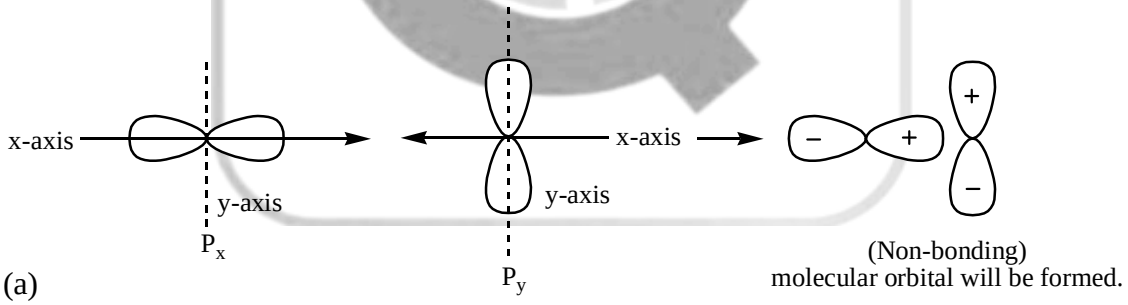
11. (c)

Sol. To satisfy nodal equation number of nodes should be same and symmetry of nodes should be identical.



12. (b)

Sol.

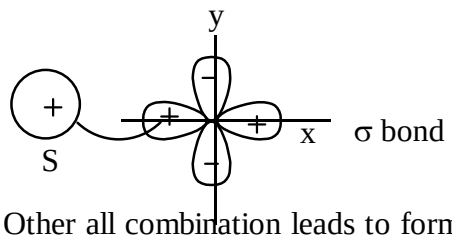


13. (a)

Sol. P_x and P_x orbital combines along x-axis to form non-bonding molecular orbital.

14. (a)

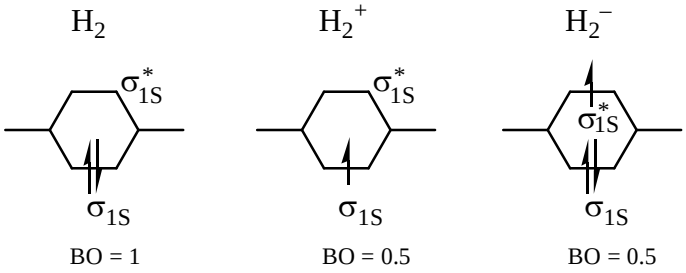
Sol.



Other all combination leads to formation of non-bonding molecular orbital.

15. (c)

Sol.



16. (b)

Sol. H_2 has both electron paired therefore diamagnetic but H_2^+ and H_2^- have 1 unpaired electron therefore it is paramagnetic.

17. (d)

Sol. F_2 is least intense and considered as colourless due to high energy transition but Cl_2, Br_2 and I_2 are coloured.

18. (c)

Sol. $$\text{Bond order} = \frac{[\text{Number of electrons in bonding molecular orbital}] - [\text{Number of electron in antibonding molecular orbital}]}{2}$$

19. (b)

Sol. The bond length is inversely proportional to the bond order, the correct order is

$O_2^{2-} > O_2^- > O_2 > O_2^+$

20. (c)

Sol. The order of stability is directly proportional to bond order. Therefore, the correct order of stability is $N_2^{2-} < N_2^- < N_2^+ < N_2$

21. (d)

Sol. Oxygen is paramagnetic in nature and its bond order is 2. It can be explained on the basis of molecular orbital diagram.

22. (c)

Sol. Molecular orbital electronic configuration of He_2 molecule = $(\sigma_{1S})^2 (\sigma^*_{1S})^2$. Bond order = 0, So He_2 molecule does not exist.

23. (b)

Sol. This order is observed when s-p mixing is observed in molecular orbital diagram. s-p mixing is possible for H_2 to N_2.

24. (b)

Sol. $$\text{Bond order} = \frac{10-4}{2} = 3$$

25. (c)

Sol. Filling of electron in case of O_2^- take place in such a way

$\sigma_{1s}^2, \sigma^{*2}_{1s}, \sigma_{2s}^2, \sigma^{*2}_{2s}, \sigma_{2p_z}^2, \pi_{2p_x}^2 = \pi_{2p_y}^2, \pi^{*2}_{2p_x} = \sigma^{*2}_{2y}$

So, last electron goes in $p^*_{2p_x}$ orbital.

26. (c)

Sol. Bond order of O_2 is 2 and in case of O_2^+ an electron in removed from anti-bonding molecular orbital therefore bond order is increased and bond length will be minimum.

27. (b)

Sol. O_2 molecules is paramagnetic as it has unpaired electron in p* (antibonding pi orbital).

28. (d)

Sol. In molecular orbital diagram of O_2 two unpaired electron are present in antibonding pi orbital is responsible for paramagnetic behaviour.

29. (a)

Sol.

Molecule	Bond order
N_2	3
O_2	2
O_2^+	2.5
H_2	1

30. (b)

Sol. Filling of electron in case of N_2^- take place as

$(\sigma_{1s})^2 (\sigma^*_{1s})^2 (\sigma^*_{2s})^2 (\pi_{2p_x})^2 = (\pi_{2p_y})^2 (\sigma_{2p_z})^2 (\pi^*_{2p_x})^2$

The lst electro enters in antibonding π molecular orbital.

31. (a)

32. (a)

Sol. $(\sigma_{1s})^2 (\sigma^*_{1s})^2 (\sigma^*_{2s})^2 (\pi_{2p_x})^2 = (\pi_{2p_y})^2 (\sigma_{2p_z})^2$

It has of N_2^+ the last electron is removed from σ_{2p_z} MO, due to which bond order decreases and bond length increases.

33. (a)

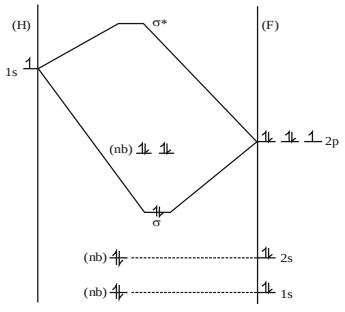
Sol. H_2^{2+} and He_2 both have zero bond order and does not exist.

34. (c)

Sol. The highest occupied molecular orbitals are non-bonding in nature comprising of 2p-orbitals of flourine.

35. (b)

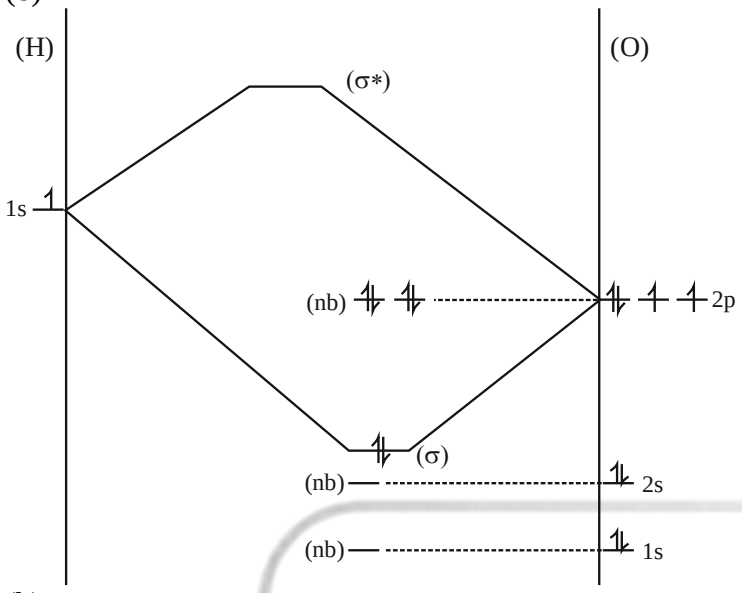
Sol.



There are total 8 non-bonding e^- i.e. 4 non-bonding e^- pairs.

36. (b)

Sol.



37. (b)

Sol. Since OH^- have two pair of non-bonding electrons so it can behave as both σ and π-donor.

38. (b)

Sol. HF and OH^- both can behave as σ-donors but only OH^- can behave as π-donor.

39. (c)

Sol. The LUMO for NO^+ is π-antibonding.

40. (c)

Sol. $\text{Bond order } \propto \frac{1}{\text{Bond length}}$

Bond order: $NO^+ > NO > NO^-$

Bond length: $NO^+ < NO < NO^-$

41. (b)

Sol. $\text{Bond order} = \frac{1}{2}[N_b - N_a] = \frac{1}{2}[10-4] = 3$

42. (a)

Sol. The bond order in OF molecule = $\frac{1}{2}[10-7] = 1.5$

43. (c)

Sol. The last electron in NO enters in π-antibonding orbitals. Therefore, on going from NO $\rightarrow$ NO^+, the electron is to be removed from π*.

44. (c)

Sol. Bond order in BF molecule is 1 because it form only one sigma bond.

45. (d)

Sol. Since both the atoms, C and N involve s – p mixing. Therefore, its MO diagram is similar to that of N_2 molecule.

46. (a)

Sol. In HF the HOMO is closer to nucleus and thereby making the donation of electrons difficult. Hence HF behaves as σ donor only.

47. (c)

Sol. CO can behave as both σ-donor & π-acceptor because it has low lying vacant π* orbitals.

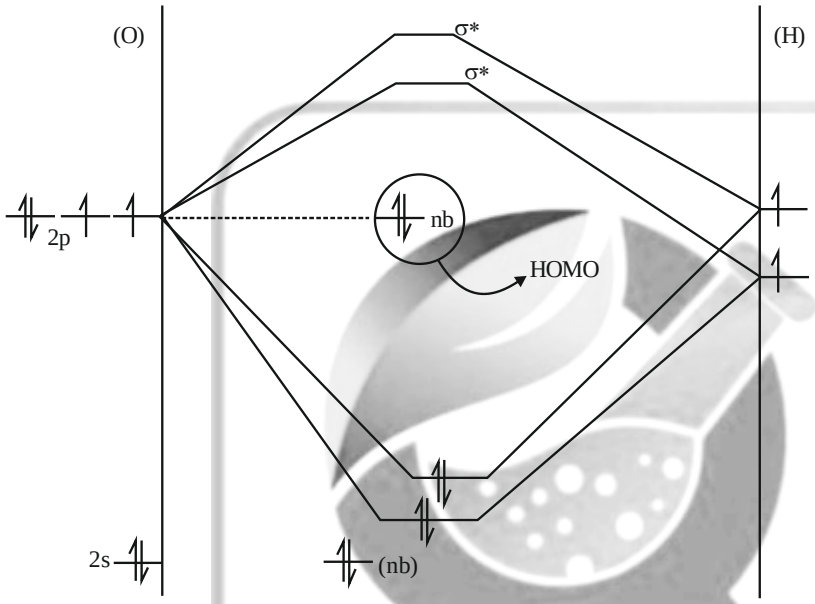
48. (c)

Sol. The MO diagram for BN will be same as that of B_2 or N_2 and as BN contain $12e^-$ and all of them will be paired.

49. (b)

Sol. The MO diagram for BN will be same as that of B_2 or N_2 and as BN contain $12e^-$ and all of the will be paired.

Sol.



50. (b)

Sol. H_2O has $2e^-$ in its HOMO while OH^- have $4e^-$ in its HOMO thereby OH^- can behave an π-donor as well.

51. (d)

Sol. N_2 and Cl_2 both involve s-p mixing as the gap between s and p-subshells is less.

52. (d)

Sol. LUMO for CO is doubly degenerate (π*) and it is of gerade symmetry.

53. (c)

Sol. Bond order of $O_2^+ = 2.5$

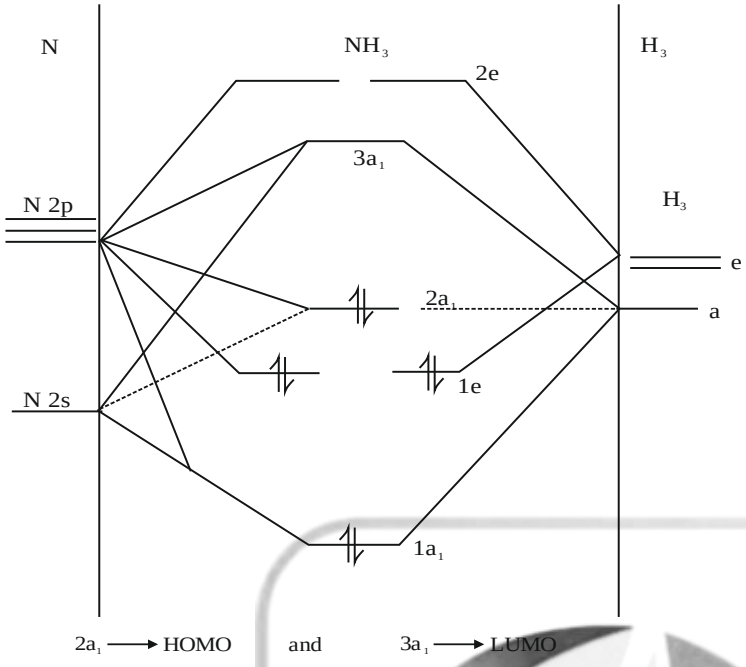
Bond order of CN: 2.5

Bond order of N_2^+: 2.5

Therefore, all three given species have same bond order.

54. (b)

Sol. The HOMO and LUMO both for NH_3 are singly degenerate.



55. (b)

Sol. The MO configuration of SF_6 is $1a_1^2\ 1t_1^6\ 1e^4$.

56. (c)

Sol. The number of unpaired e^- in O_2^-, O_2^+ are unpaired e^- in each while BN have no unpaired electron.

57. (c)

Sol. BN and O_2 have singly degenerate LUMO while CN and NO^+ have doubly degenerate LUMO.

58. (b)

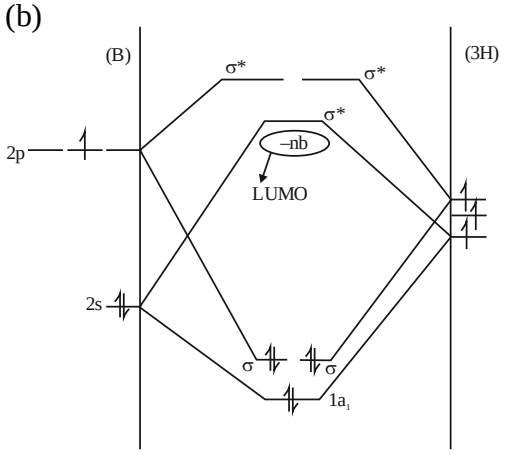
Sol. NO^+ and CO are isoelectronic because they have same no. of electrons ($14e^-$).

59. (a)

Sol. No. of e^- in NO^+ and N_2 are $14e^-$ and both have bond order 3.

60. (b)

Sol.



LUMO is of non-bonding nature.

61. (c)

Sol. The HOMO of CO_2 molecule is 2 non-bonding orbitals having $2e^-$ each. The LUMO for CO_2 is π^* orbitals (doubly degenerate)

62. (a)

Sol. HOMO of HF $\rightarrow$ non-bonding

LUMO of BF $\rightarrow$ non-bonding

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

Assignment Sheet - MOLECULAR ORBITAL THEORY

MSQ

1. Which of the following statement is true for sigma molecular orbital.
   (a) may result from overlap of p atomic orbitals perpendicular to the molecular axis (side-on).
   (b) may result from overlap of p-atomic orbitals along the molecular axis (head-on).
   (c) may result from overlap of two s-atomic orbitals.
   (d) may result from overlap of one s and one p atomic orbital.
2. Which of the following statements are true for p-orbital and σ-orbital.
   (a) p-orbital are single nuclei (b) σ* orbital are single nuclei
   (c) In p-orbital node passes through nucleus. (d) In σ*-orbital node does not pass through nucleus
3. Which of the following statements are true.
   (a) π-molecular orbitals are ungerade whereas
   (b) π-molecular orbital are gerade gerade π^*-molecular orbital are ungerade.
   (c) Sigma molecular orbitals are ungerade whereas σ* molecular orbitals are gerade.
   (d) Sigma molecular orbitals are gerade whereas σ* molecular orbital are ungerade.
4. Which of the following statements are correct.
   (a) In bonding molecular orbitals, electron density is low in the region, between the nuclei of bonded atoms.
   (b) The energy of antibonding molecular orbital is higher than that of atomic orbitals from which it is formed.
   (c) Every electron in bonding molecular orbital contributes towards stability of the molecule.
   (d) Antibonding orbitals are formed when lobes of atomic orbitals have different signs.
5. Which of the following statements are true.
   (a) Symmetry of nodes are defined with respect to internuclear axis.
   (b) Symmetry of orbitals are defined with respect to centre of symmetry.
   (c) Symmetry of delta (δ) bonding molecular orbital is gerade.
   (d) $d_{x^2-y^2}$ orbital can form delta bond but d_{xy} orbital cannot form delta bond.

6. Which of the following statements are true
   (a) s orbital and σ-molecular orbital symmetrical
   (b) p orbital, σ* and π molecular orbital are ungerade.
   (c) f atomic orbital have 3 nodes
   (d) ϕ* molecular orbital have 4 nodes
7. Which of the following statements are correct.
   (a) $d_{x^2 - y^2}$ and $d_{x^2 - y^2}$ orbital combine along x-axis to form sigma bond.
   (b) $d_{x^2 - y^2}$ and $d_{x^2 - y^2}$ orbital combine along z-axis to form sigma bond.
   (c) d_{xz} and d_{xz} orbitals combine along y-axis to form δ-bond.
   (d) d_{xz} and d_{xz} orbitals combine along y-axis to form π-bond.
8. If x is considered as internuclear axis, then which of the following overlapping is/are for the formation of Non-bonding molecular orbital.
   (a) $P_x + P_y$ (b) $P_y + P_z$ (c) $P_x + P_x$ (d) $P_z + P_x$
9. Which of the following statements is/are true.
   (a) P_z and d_{z^2} orbitals combine along x-axis to form π-bond.
   (b) P_z and d_{z^2} orbitals combine along x-axis to form non-bonding molecular orbital.
   (c) When two d_{z^2} orbitals combine along x-axis to form π-bond.
   (d) All of these
10. If x is internuclear axis, then which type of overlapping is/are responsible for the formation of non-bonding molecular orbital?
   (a) $d_{xy} + P_x$ (b) $d_{xy} + S$ (c) $S + P_y$ (d) $S + P_z$
11. If x-axis is considered as internuclear axis which type of overlapping is/are responsible for the formation of π-bond.
   (a) $P_y + d_{xy}$ (b) $d_{xy} + d_{xy}$ (c) $d_{x^2 - y^2} + d_{x^2 - y^2}$ (d) $d_{z^2} + d_{z^2}$
12. Filled MO diagram provide information about:
   (a) Bond order (b) Frontier orbital (c) Magnetic nature (d) Nature of ligand
13. Which of the following statements are correct.
   (a) order of bond length $H_2 > H_2^+ > H_2^-$ (b) order of bond length $H_2 > H_2^+ = H_2^-$
   (c) order of bond length $H_2 > H_2^- > H_2^+$ (d) order of bond length $H_2 > H_2^+ = H_2^-$
14. Which of the following molecules does not exist according to molecular orbital theory.
   (a) He_2 (b) C_2 (c) B_2 (d) N_2
15. Which of the following molecules/ions have same bond order.
   (a) O_2 (b) N_2^{2-} (c) H_2 (d) N_2^-
16. Mark the correct statement regarding Li_2.
   (a) The bond order of Li_2 is 1
   (b) The last two electrons enters in bonding orbital.
   (c) Li_2 contain 8 electrons.
   (d) None of these

17. How many of the following is/are diamagnetic.
C_2^{2+}, C_2^{+}, C_2, C_2^{-}, C_2^{2-}

18. The correct statement(s) among the following are—
(a) CN^- and N_2 are isoelectronic
(b) CN^- and N_2 have same bond order
(c) The structure of MO diagram is same for both CN^- and N_2
(d) All the given statements are correct.

19. Consider the following statement(s) and mark the correct–
(a) NO and OH^- are not isoelectronic.
(b) HF and OH^- have bond order approximately equal to 1.
(c) There are total two non-bonded e^- pairs in OH^-.
(d) OH^- is both σ donor & π-acceptor.

20. Among the following, the correct statement(s) are–
(a) CO and CN^- are isoelectronic
(b) Bond length of N – O in NO^+ is greater than NO.
(c) CO behave as π-acceptor only
(d) MOT can predict π-acceptor & π-donor behaviour of any specie.

21. Predict the correct statement(s) among the following–
(a) the bond order of BN is 2.
(b) NO is paramagnetic in nature
(c) CO and NO^+ are isoelectronic
(d) The LUMO of B_2 is of gerade symmetry

22. The incorrect statement(s) among the following—
(a) The polyatomic molecules formation is explained by the concepts of LGOs in MOT.
(b) Hybridization is a concept of MOT.
(c) For atomic orbitals to undergo mixing to form molecular orbitals they should belong to same atom.
(d) The bond order of O_2^{2+} and N_2 is same.

23. The correct statements(s) among the following—
(a) The bond order of CO and NO^+ is same.
(b) Bond length: $N_2 < N_2^{+} < N_2^{2+}$
(c) Bond length: $N_2 > N_2^{+} > N_2^{2+}$
(d) π-donor and π-acceptor behaviour can be explained by MOT.

NAT

24. In how many of the following s-p mixing will be favourable.
HF, F_2, Br_2, Cl_2, CO, NO, BF, NF, OF, C_2,

25. In how many of the following s-p mixing will not be favourable.
O_2, BO, FNen, CNe, CN^-, HCl, HBr, OH^-

26. How many orbitals from the following will remain same after a rotation through 180°.

σ, π, π^*, d

27. Overlapping of how many lobes of orbital is required for the formation of ϕ bond.
28. How many nodes are present in delta (δ) antibonding molecular orbital.
29. Total number of electrons in anti-bonding MO in O_2^- (superoxide ion) is .....
30. The number of molecules having bond order approximately equal to 3 are–
    CN^-, BF, NO^+, N_2, OH^-, F_2
31. The molecules having LUMO of ungerade symmetry are–
    O_2, N_2, B_2^{2+}, CO, CN^-
32. The number of species isoelectronic with BN are–
    C_2, N_2^{2+} , O_2, HF, H_2O
33. The species having bond order equal to NO^+ are—
    CO, N_2, O_2^{2+}, C_2^{2-}, O_2, F_2

×××××

QUANTA CHEMISTRY

An Institute of Chemical Sciences

ANSWERS

1. (b, c, d)
2. (a, c, d)
3. (a, d)
4. (b, c, d)
5. (a, b, c)
6. (a, b, c, d)
7. (a, b, d)
8. (a, b, d)
9. (b, c)
10. (a, b, c, d)
11. (a, b, d)
12. (a, b, c, d)
13. (a, d)
14. (a, c)
15. (a, b)
16. (a, b)
17. 2
18. (a, b, c, d)
19. (a, b, d)
20. (a, d)
21. (a), (b), (c), (d)
22. (b) & (c)
23. (a), (b), (d)
24. 6
25. 4
26. 3
27. 6
28. 3
29. 7
30. 3
31. 2
32. 2
33. 4

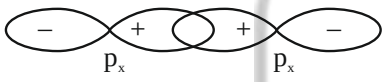
QUANTA CHEMISTRY

An Institute of Chemical Sciences

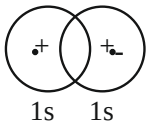
Hints & Solutions

1. (b, c, d)

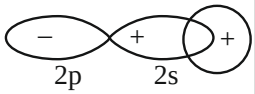
Sol. When p-orbitals overlap along molecular axis sigma bond is formed by head on overlap.



Two s-orbitals combine to form sigma bond.

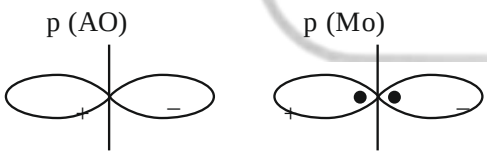


One s and one p-orbital may overlap to form sigma bond.



2. (a, c, d)

Sol. p-orbital is a atomic orbital therefore have single nucleus. Whereas σ* is molecular orbital.



In atomic orbitals nodes passes through nucleous, but in molecular orbitals nodes does not pass through nucleous.

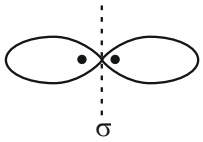
3. (a, d)

4. (b, c, d)

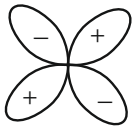
Sol. In bonding molecular orbitals, the electron density is high in the region between the nuclei of bonded atoms. All the other options are correct. Thee energy of antibonding molecular orbital is higher than that of atomic orbital from which itis formed. Every electron of molecule. Antibonding orbital is formed when lobes of atomic orbitals have different signs.

5. (a, b, c)

Sol. Symmetry of nodes are defined with respect internuclear axis.

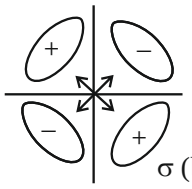


Symmetry of orbitals are defined with respect to centre of symmetry.



→ centre of symmetry present (gerade)

Symmetry of delta bonding molecular orbital is gerade



σ (bondindg)

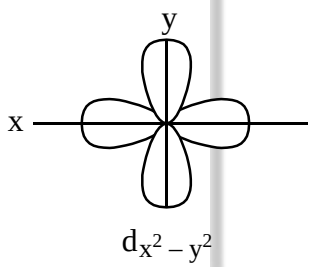
gerade

$d_{x^2-y^2}$ and d_{xy} both can form delta bond.

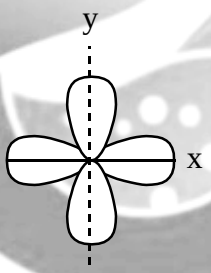
6. (a, b, c, d)

7. (a, b, d)

Sol.



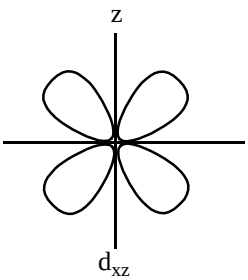
$d_{x^2-y^2}$



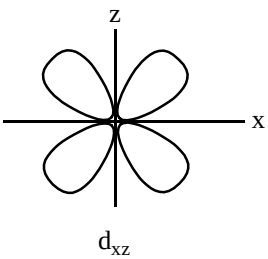
$d_{x^2-y^2}$

one lobe will interact to form sigma bond along x-axis.

When two $d_{x^2-y^2}$ orbital combine along z-axis, four lobe-four lobe interaction take place and δ bond is formed.



d_{xz}



d_{xz}

When two d_{xz} orbital combines along x-axis to form π-bond as two lobe-twop lobe interaction takes place.

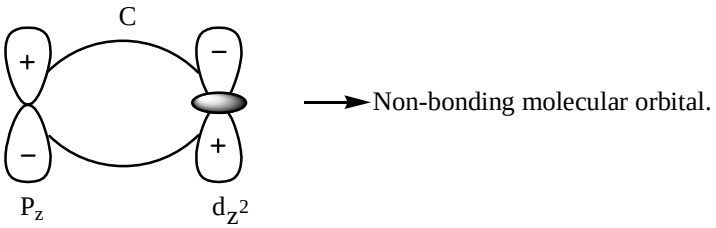
The combination of two d_{xz} orbital along y-axis to form δ-bond is not possible practically.

8. (a, b, d)

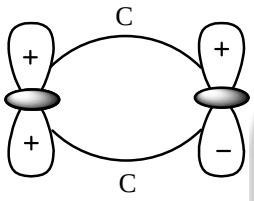
Sol. When two P_x orbitals combine along x-axis σ bond formation will taken place.
Other all the above combination will form non-bonding molecular orbital along x-axis.

9. (b, c)

Sol.



Two d_{z^2} orbitals combine along x-axis to form π-bond.



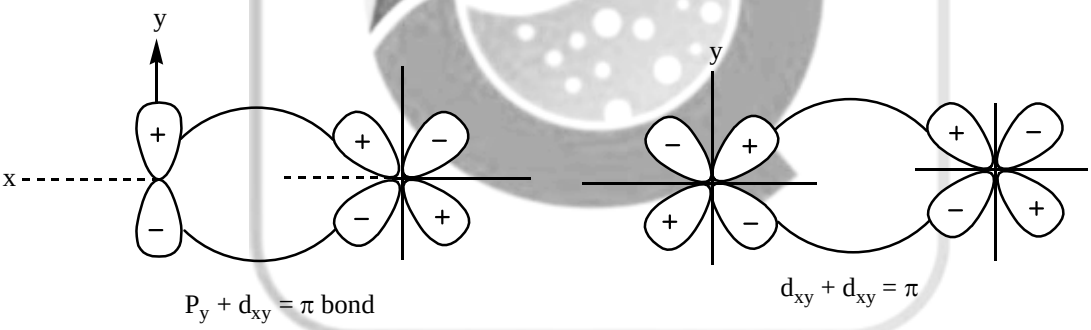
Bonding π-molecular orbital.

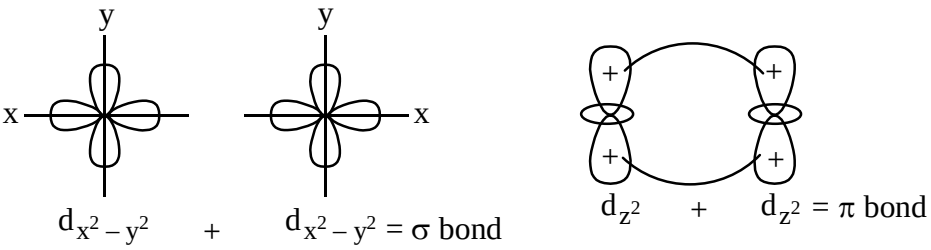
10. (a, b, c, d)

Sol. All of the following combination will form non-bonding molecular orbital.

11. (a, b, d)

Sol.





12. (a, b, c, d)

Sol. All the above properties can be explained by filled MO diagram.

13. (a, d)

Sol. Bond length is inversely proportional to bond order. But if bond order is same then the species having greater number of electron will have greater bond length.

14. (a, c)

Sol. According to the molecular orbital theory bond order of He_2 and B_2 is zero.

15. (a, b)

Sol. O_2 and N_2 have same bond order equal to 2.

16. (a, b)

Sol. $(\sigma_{1s})^2\ (\sigma^*_{1s})^2\ (\sigma_{2s})^2$

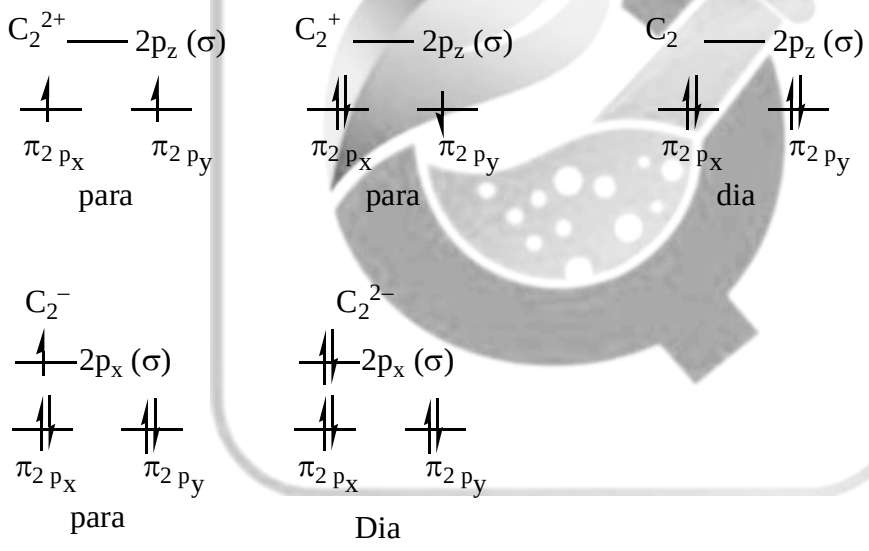
the last two electrons enter in bonding molecular orbital.

$$\text{Bond order} = \frac{\frac{1}{2}[\text{No. of bonding electrons-No. of antibonding electrons}]}{2}$$

$$= \frac{1}{2}[4-2] = 1$$

17. 2

Sol.



C_2 and C_2^{2-} are diamagnetic.

18. (a, b, c, d)

Sol. CN^- and N_2, both have $14e^-$ bond order is 3 for both. Both involve s – p mixing, therefore same structure of MO diagram.

19. (a, b, d)

Sol. • NO and OH^- are not isoelectronic.

• There are total 4 non-bonded e^- pairs in OH^-.

• OH^- is σ-donor & π-donor.

20. (a, d)

Sol. • Bond length of NO: $NO^+ < NO$

• CO is both σ-donor & π-acceptor.

21. (a), (b), (c), (d)

Sol. • Bond order of BN is 2

• NO has are unpaired e^- hence paramagnetic.

• CO and NO^+ both contain $14e^-$ hence isoelectronic

• LUMO of B_2 is σ which have gerade symmetry

22. (b) & (c)

Sol. Hybridization is a concept of VBT.

• For atomic orbitals to form molecular orbitals, they should be of almost same energy, same symmetry and belong to different atoms.

23. (a), (b), (d)

Sol. • Bond order of CO and NO^+ is 3

• Bond length $\alpha \frac{1}{\text{Bond order}}$

24. 6

Sol. Br_2, Cl_2, CO, NO, BF, C_2

If mixing is favourable is one of the atom we consider that mixing will be favourable in the molecule.

25. 4

Sol. FNE, ONe, OH^- will not undergo s-p mixing.

26. 3

Sol. σ, π* and d orbitals are gerade and will remain same after a rotation through 180°.

27. 6

Sol. If six lobes of one orbital overlap with six lobes of other orbital the ϕ bond is formed.

28. 3

29. 7

Sol. O_2^- (17 electrons) has molecular orbital electronic configuration.

$(\sigma_{1s})^2, (\sigma^*_{1s})^2 (\sigma_{2s})^2 (\sigma^*_{2s})^2 (\sigma_{2p_z})^2 (\pi_{2p_x})^2 = (\pi_{2p_y})^2, (\pi^*_{2p_x})^2, (\pi^*_{2p_y})^1$

Underlined are antibonding molecular orbital. Thus, seven electrons are in anti-bonding molecular orbitals.

30. 3

Sol. CN^-, N_2, NO^+ have B.O. ≈ 3.

31. 2

Sol. O_2, B_2^{2+} have LUMO of ungerade symmetry. They are σ* & π respectively.

32. 2

Sol. C_2 and N_2^{2+}

33. 4

Sol. CO, N_2, O_2^{2+}, C_2^{2-}

××××××